PHILIPS

Crystal

Position	Type	Part #
1	LiF <200>	PW 1530/30
2	PET	PW 1535/30
3	LiF <220>	PW 1538/30
4	TAP	B00-129-01
5		
6		

Mask

Position	Diameter
1	35 MM
2	24 MM

1. BASIC INSTRUMENT-OPERATION

The operation of the basic instrument is simple – manual controls are virtually eliminated, and analysis is controlled from a typewriter keyboard. Sets of measurement parameters are stored, and a microprocessor controls the measurement and output to a printer and/or visual display unit. The microprocessor control diagram is shown in figure 1A.

The measured intensity data can be further processed by a programmable desk calculator or a computer, and the operation and software when the Philips P851 minicomputer is connected is described in paragraph 2. Note that the software descriptions use the term "parameter bank" to indicate the area used for storage of parameters in the microprocessor (basic) version, and the term "databank" for the parameter and data storage area in the P851 (or other) computer.

The simplified operation procedure described in paragraph 1.1. is intended for use by non-specialist personnel, who are only required to load the sample and to select a measuring program (or job) already stored in the parameter bank. This simple procedure will also apply when a computer is connected. The paragraphs that follow describe the preparation of measuring and job programs, and the selection of the spectrometer control parameters.
In the event that operation is not possible, check the Operation Notes (paragraph 1.1.).

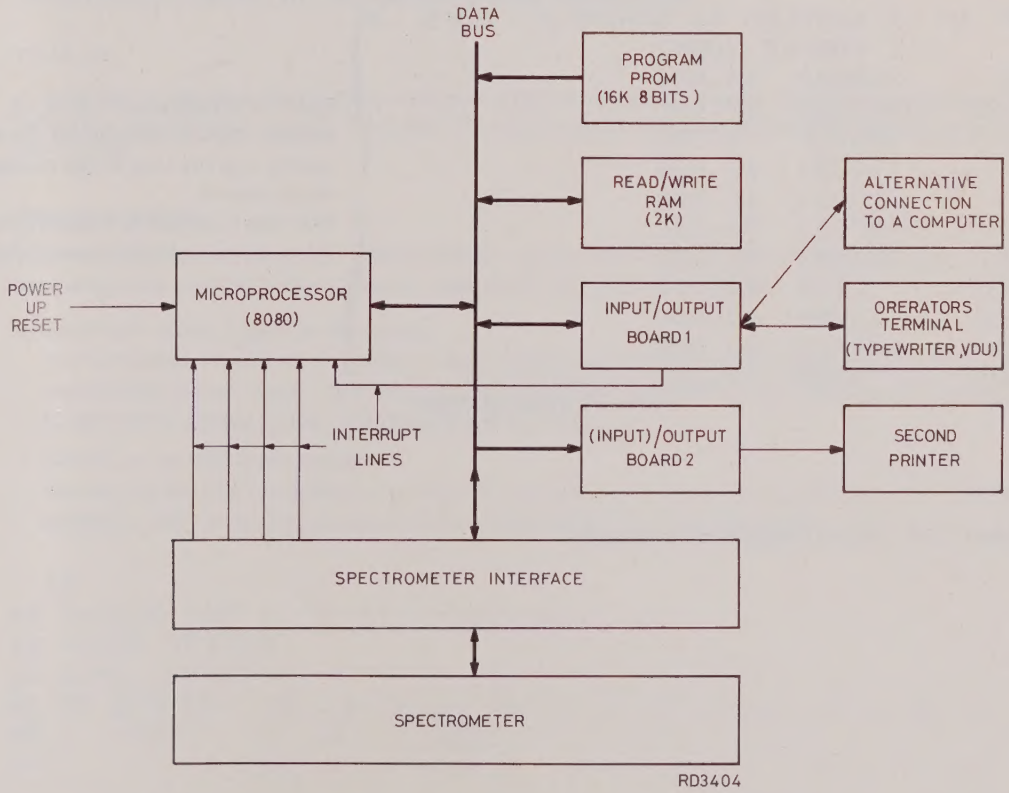


Figure 1A PW1400 Microprocessor control diagram

1.1. SIMPLE OPERATION PROCEDURE

This procedure assumes that the spectrometer controls, such as detector H.T., have been correctly set, and the instrument and measurement parameters have been input i.e. ACH, AMP lists in the parameter bank, PWR and SPN input. Also, the spectrometer medium (vacuum, helium or air) is selected - see paragraph 1.6.5.

System in the standby condition (switched on but no X-rays)

- Check that the H.T. generator kV and mA controls are in the minimum position
- Operate the HIGH VOLTAGE I push-button (if H.T. is not generated check the water flow and safety circuit operation).

System ready for operation (X-rays present).

- Prepare samples and place in sample holders.

Analysis of samples.

- Type RCM or RCJ, if required (recycle commands)
- Type start measurement command (c.r., 1-63, SMX or SJB)
- Load sample(s), and give identification. The procedure will depend whether the batch (BMD) or continuous (CMD) mode has been selected previously - see paragraph 1.4.5.
- Give SLP command to unload the sample (batch mode)

The resultant output from a typical sample measurement is shown in figure 1.1A.

```
C=10                          Measurement program 10 selected for sample measurement
SAM.POS  :=4  I               Sample to be placed in turret position 4, and to be identified
<4>  :=SAMPLE  IDENT          Sample identification input
                              Sample to measuring position and measurement commences
MP  10   1  SAMPLES  11  CHANNELS   MOPS   0
      4  :  SAMPLE  IDENT
FE        218447    10.000
CA2      5065738    20.000
K         383276     4.000
S         170754    10.000
S+         10074    10.000
SI        947083    20.000
AL        224862    20.000
MG2-        2103    20.000
MG2        21859    40.000
NA         32671    40.000
NA+         5375    20.000
C=                            Ready for a new command
```

Result of measurement (showing element channel designation, the total counts, and the time of the channel measurement).
This data is output to a second printer, if connected and SOT command given.

Figure 1.1A Simple measurement of a sample

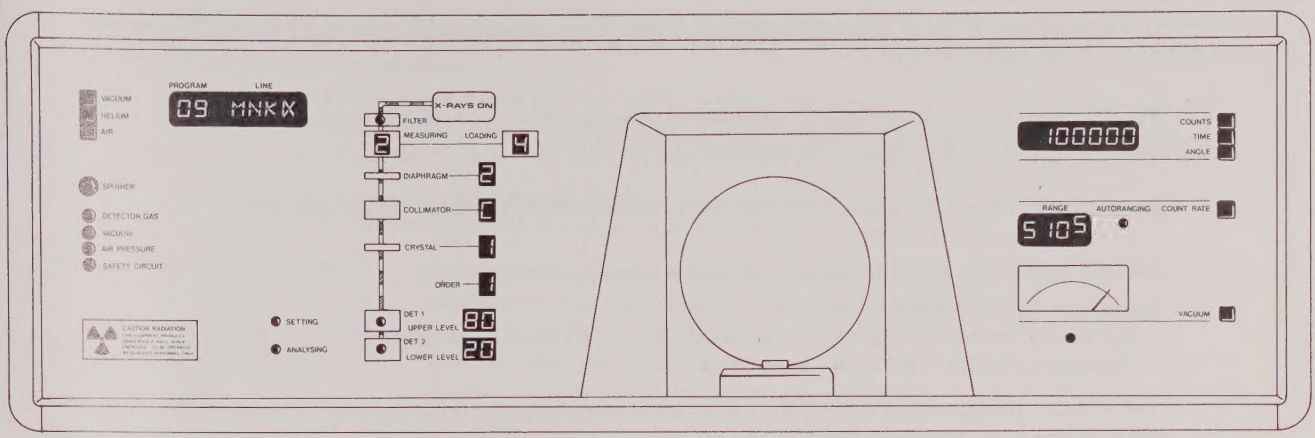


Figure 1.1B Spectrometer front panel controls

1.1.1. Operation notes.

These notes draw attention to features of the spectrometer and its operation which are relevant during installation, start up, program assembly and sample measurement. The examples shown in the manual use shading to indicate operator input data. Also see paragraph 2.1.1. when a computer is used.
READ BEFORE USING THE PW1400 SPECTROMETER SYSTEM.

Check list.

A check list of essential requirements is given in Appendix A, and will apply during the installation period and before the spectrometer is used. Thereafter the operation will be in accordance with the relevant paragraphs in this manual.

Start up procedure.

When the electrical power, water, compressed air, gas supplies, and terminal device(s) have been correctly connected (and adjusted where necessary - see check list), proceed as follows:

– *Switch on - mains supply to the system.*
The temperature stabilisation system in the spectrometer cabinet is active (cooling water flow on), and the spectrometer power supplies will now maintain the data in the memory and recharge the standby battery (if BATTERY switch is ON). The detector gas will flow.

– *Switch on - system mains supply.*
Operate the MAINS I push-button in the H.T. generator front panel. The system is now in a **standby condition**, and the microprocessor initiation program will run, and then output:

```
  **
** PW1400 (VS 1.1) TEST PROCEDURE
** PROMS TESTED
** RAMS TESTED
** HW STATUS : 51 16 00 EA 00 7F FF 83 82 82 82 82 82
**     .000          0     .000
C=
```

Figure 1.1C Start up readout

This output may vary slightly, depending on the software program reference and the instrument conditions, but if an error message is printed refer to the Service Manual.

It is now possible to input software commands, except these requesting H.T. generator settings (kV and mA) such as SMX, SCH, KVM,etc.

Type the PWR i k command, where i = maximum power to the X-ray tube (kW value up to the tube maximum), and k = kV rating of the generator (60 or 100 kV).

At switch on, or reset, the spinner will run. Use command SPN N to switch off (if required).

Set MSK (collimator mask) as required, for details refer to paragraph 1.6.3.

Switch on - H.T. generator

Set the kV and mA controls to the minimum position on the H.T. generator.
Operate the HIGH VOLTAGE I push-button.

The X-RAYS ON lamps will light, and the main water cooling system is switched on, i.e. water flows through the X-ray tube, etc. Using the 100kV generator, it is good practice to gradually apply H.T. to the tube by setting the kV to 60 for 5 minutes before applying a higher voltage.
List and program assembly is possible, and spectrometer operation is normal, as described in the following paragraphs.

Reset

– If the RESET push-button on the spectrometer side panel is operated, the microprocessor initiation program is restarted, and the output (as shown above) is printed or displayed. The parameter bank is not affected.

Switch off - H.T. only

Operating the HIGH VOLTAGE 0 push-button will switch off the generation of H.T., and the system is now in a **standby condition.**

Do not switch off the H.T. if high precision analysis is required inmediately after a period of non-use (overnight or weekend). In this case set the generator to 50kV and 40mA when not in use. Alternatively, set to 50kV and 10mA if a stabilisation period of about half an hour is acceptable before analysis. Also refer to paragraph 6.5.1.

Switch off

Operate the MAINS 0 push-button.
DO NOT DISCONNECT FROM ELECTRICAL MAINS SUPPLY OR TURN OFF WATER SUPPLY - unless the cabinet temperature stabilisation is not required.

Turn off - electrical mains and water supply

In addition to the above actions, disconnection of the mains supply will cause the memory data to be maintained by a battery on the bus interface card. A **fully charged** battery will protect the data for 500 hours - refer to paragraph 1.3.4.

Software notes.

The following symbols are used as identification:

** Microprocessor generated error message
*** Computer generated error message
* means that computer dialog is selected.
C = means that a microprocessor command can be input
J = means that a job is being assembled and only permitted commands can be input. To revert to C = dialog give an end of job assembly (EJB) command.

c.r. used in the following description means carriage return. If a c.r. is given alone, this is recognised as a start measurement command, see paragraph 1.4.1., and the first or the previously input MP list will be used, A slash (/) is used as a stop command.

Error correction

The correction of typed (input) characters, or a line of input data, is possible **provided that a carriage return has not yet been given.** When the PC 1409/00 printer or P817 - 001 VDU (or similar terminal) is connected the following deletion commands can be given:

- To delete a character type a long dash (—), which is upper case minus sign (PC1409) or upper case zero (P817). This deletes the previously typed character, and the correct character can now be input. More than one character can be deleted by typing a dash for each of the previously input characters.
- A whole line of data can be deleted by typing a ∧ plus c.r.∧ is upper case 6 (PC1409) or lower case ~ (P817). The correct data can now be input before giving a carriage return.

```
C=PTS 2_10          Deletion of one character (change from 2 to 10 seconds)
C=CCT___SCT         Deletion of three characters (CCT replaced by SCT)
 57.520   3562649   10.000
C=PTS 40^           Deletion of complete line
SCT                 Replaced by new command (SCT replaces PTS 40)
 57.520   3563987   10.000
C=
```

During list assembly the microprocessor will recognise an incorrect input when the carriage return is given, and an error message will be printed, see paragraph 1.2.1. The correct answer must then be input.

```
C=AFM               Incorrect command (deliberately input)

** ERROR  COMMAND NOT AVAILABLE
C=AMP 382           Incorrect argument input

** INVALID ARGUMENT
C=AMP 3

MASK :   1 :=
ABS  :  YE :=       Carriage return given as value not changed

CHAN    PT    PC
          0   0E0 :=FE 1E6 10      Preset count given before preset time

** INVALID, CORRECT VALUE(S) =FE 10 1E6   Correct values/order input
          0   0E0 :=NI 20 1E6      Dialog moves to next input
          0   0E0 :=
                    /              Terminate assembly
C=                                 Ready for a new command
```

Figure 1.1D Deletion and error message operation

During the input of commands, or during list assembly, a comma (,) can be typed instead of a space or instead of argument characters. The comma is recognised as "skip argument", and will not cause an error message unless the argument is mandatory.

Analysis identification input

The printer can be used off-line to type any data in the normal manner, but data can also be typed on-line, for example, to give sample batch analysis details, program identification, etc. These data can be input after the last argument of a command, and before the carriage return is given. Only the command and the argument will be recognised by the microprocessor.

Use the COM command when output of operator typed input to a second terminal is required, see paragraph 1.5.

The maximum number of characters that can be typed on one line is 80, which includes command, arguments, spaces and supplementary information.

1.2. SURVEY OF COMMANDS

The PW1400 microprocessor version (basic instrument) is programmed to accept the commands listed in this paragraph, and will generate error messages in the event of incorrect operation. Additional commands can be given when the P851 M minicomputer is connected, and these are described in paragraph 2. A complete listing of the microprocessor and minicomputer commands, in alphabetical order, is included in this paragraph.

When the PW1400 is switched on (at the H.T. generator), the printer will type a test procedure routine, and then C = when the system is ready to accept a keyboard command. A command must be given before any further operation is possible, and the following information should be noted:

- Commands are three letter abbreviations (except stop commands)
- Commands can be followed by one or more arguments, each separated by a space (or comma)
- Commands must be terminated by a carriage return, after the last argument is given, and then the required action is initiated.
- The command listing shows the range of an argument thus: SMX i, where i must be a number from 1 to 63.
- Optional arguments are shown between brackets thus: SMX i (j) (k), means that the number for i is mandatory, but j and k are only given if required.

Measurement commands

COMMAND/ARGUMENT	MEANING
■ SMX i (j)(k)	Start measuring unknown samples, using measuring parameter list (MP) i, and j and k if required. i (j and k) = 1 to 63. Give a space between arguments. See also paragraph 1.4.
▲ SMM i (j)(k)	Start measuring monitor sample, using measuring program i, j, k. i, j, k = 1 to 63.
SJB i	Start measurement using the job program i. i = 1 to 63
RCM i	Recycle the measurement program i times given before a start measurement command. i = 0 to 127. 0 means infinity. Refer to paragraph 1.4.6.
RCJ i	Recycle job progam i times (before SJB). i = 0 to 127 Refer to paragraph 1.4.8.
MPY i	Multiply the preset time and preset count values i times, where i = 1, 2, 4, 10, 20 or 40. The PT and PC values are those shown in the MP lists. Refer to paragraph 1.4.6.
RES	Resets all RCM, RCJ, MPY, ASC and RCS commands. The individual commands are also effectively reset when i = 1, except ASC.
■ CAN xxi	Calibrate the angle of channel xxi, where xxi is the name of the channel - see ACH command. Refer to paragraph 1.4.10.
PHD (xxi)	Pulse height distribution readout of the channel xxi, where xxi is the name of the channel - see ACH command. Refer to paragraph 1.4.11.

■ Means that the command can be assembled in a job list (AJB), and the job measurement commences from the SJB command or by selection from a sample changer tray identification card.

▲ Means that the command can be included in a job list, but the list cannot be selected from a sample changer card.

COMMAND/ARGUMENT	MEANING
CMD	Continuous mode measurement. The cap is open during the measurement of a previously loaded sample, and this allows the continuous loading and measurement of samples. Turret positions 2 and 4 are used. Refer to paragraph 1.4.5.
/C	In continuous mode cap closes and sample passes through airlock.
BMD	Batch mode measurement. Samples are loaded into turret positions 1 to 4, before measurement, and the cap remains closed until all results are printed.
Assembly	
ACH	Assemble a new channel. The order of the readout of channel data is the same order in which the channels sets are assembled.
ACH (xxi)	Assemble or change the parameters of channel xxi. The first x of a channel name must be a letter, and can be followed by an optional letter and/or a number. Up to 63 channels can be assembled. See figure 1.3A.
PCH	Print all channel data, in blocks of 5 channels, see figure 1.3B.
PCH xxi	Print the parameters of the specified channel.
AMP i	Assemble a measurement parameters list number i, where i = 1 to 63. See figure 1.3C.
PMP i	Print the measurement parameter list number i.
DMP i	Delete the measurement parameter list number i from the memory.
AJB i	Assemble a job measurement program number i, where i = 1 to 63. Refer to paragraph 1.3.3.
DJB i	Delete the job measurement program number i from the memory.
EJB	End of a job measurement program to terminate J = input (revert to C =)
PPB	Print the contents of the parameter bank, to show the channel names, numbers of the MP lists and JB lists, and the remaining free space (in words) in the memory.
PPB a	Print the specified part of the parameter bank, where a = C to show list of channels a = M for MP list numbers a = J for job list numbers a = F for free space only.
DPB	Dump the parameter bank data into the printer, or other device (tape punch, floppy disc, etc.) if connected and selected, to preserve a record if the parameter bank is to be cleared. The RPB command is used to read the data back into the memory.
RPB	Read the data from an external storage device into the parameter bank.
CPB	Clear all data from the parameter bank.

Parameter setting

- SCH xxi (b) — Set the parameters of the channel list xxi into the spectrometer, where xxi = as SMX command, and b = + or − (offset in degrees 2 θ). Note — a space must not be given between xxi and b.
- XTL i — Set crystal changer to the position i, where i = 1 to 6.
- ORD i — Set the order of reflection to i, where i = 1 or 2.
- COL a — Set the collimator to position a, where a = F (fine), or a = C (coarse).
- FLT a — Set the beam filter to a, where a = Y (yes - filter in), or N (no - filter out).
- MSK i — Set the mask to position i, where i = 1 or 2
- DET a — Select detector a for counting, where a = F (flow detector), or S (scintillation detector), or FS (both detectors).
- LWL i — Set the lower level value of the window to i, where i = 0 to 99 (%) in 1% steps.
- UPL i — Set the upper level value of the window to i, where i = 0 to 99 (%) in 1% steps, and 0 means infinity. If UPL $\leqslant$ LWL, the window is set to zero.
- KVM i j — Set the H.T. generator output to i kV and j mA, where: i = 25 to 100 kV in 5 kV steps, and j = 10 to 80 mA in 5 mA steps. If the product i times j, or the value for i, are greater than the kilowatt and kilovolt values given in the PWR command, the operation is inhibited and the error message INVALID ARGUMENT is generated. At 25kV the maximum mA is 65.

Goniometer operation

- SLF x — Slew fast to angle x, where x = 0 to 147 ($^{o}2\theta$) in 0,005^{o} steps, using the angle approach loop operation.
- SLS x — Slew with slow speed to angle x, where x as SLF, without using the angle approach loop.

SSM ss — Single step mode with steps of ss ($^{o}2\theta$), where ss = 0,005 to 0,635 in multiples of 0,005^{o}. Refer to paragraph 1.4.9. for operation e.g. to reverse direction or change step size.

- STS x ss — Step scan from existing goniometer angle to angle x (x as SLF command), with ss degrees per step (ss as SSM command). The measurement time per step is determined by the PTS (or PCS) command, given before the STS command.
- CTS x s — Start a continuous scan to angle x (x as SLF command), with a goniometer speed of s$^{o}2\theta$ per minute, where s = 0.25, 0.5, 1.0, 2, 4, 8, 16 or 32.

Counter/Timer

- PTS t — Set preset time to t seconds, where t = 0 to 999.9 in steps of 0.1. If t = 0 the time is set to infinity.

The PTS, PCS, and PTC command values remain active until changed to another value.

■ PCS iEj	Preset count setting to iEj counts, where i = 1, 2, 5 or 0 (0 = off i.e. infinity), E stands for Exponential and j = 4 to 7. Thus, the preset count range is 1E4 to 5E7, i.e. 10 000 to 50 000 000.
■ PTC t iEj	Preset time and count setting, where t = as the PTS command, and iEj = as the PCS command. Sample measurement using this command will stop when the first condition (counts or time) is reached.
■ SCT	Start counter/timer, e.g. for manual measurement of a sample.

Instrument conditions

PWR i k	The maximum values of the power (i) and voltage (k) of the H.T. generator are defined, where i = 0 to 3 (kilowatts) in 0.1 steps, and k = 60 or 100 (kilovolts) – for the PW 1730/10 or the PW 1732/10 generator.

The command must be given when the PW1400 is first switched on, and remains active provided mains or battery power is on the RAM card.

■ MSK i	Select collimator mask position i, where i = 1 or 2. Refer to paragraph 1.6.3. for mask details
SPN a	Set spinner to condition a, where a = Y (yes = on) or a = N (no = spinner off).

Output devices

NRL i	Number of lines i per page, where i = 0 to 24, and 0 means a continuous display. Refer to paragraph 1.5.2.
SOT a	Print the measurement result to a second output terminal (printer or other device), where a = Y (yes) or a = N (no second printer output).
COM	Communication to a second printer of non-measurement data. Refer to paragraph 1.5.
■ RMS iEj	Set the ratemeter (chart recorder) to full-scale range iEj, where i = 1, 2, or 5,or 0 to give automatic ranging, E = exponential, j = 2 to 5. Therefore, range can be set from 100 to 500 000.

Sample loading

SLP i	Turret sample position i to loading position, where i = 1 to 4. Cap is open.
▲ SMP i	Turret sample position i to measuring position, where i = 1 to 4. Cap is closed.
▲ LDM i	Load monitor sample in turret position i, where i = 1 to 3 (BMD), 1 and 3 (CMD).
▲ ULM i	Unload monitor sample in turret position i, where i = 1 to 3. Cap is open.

Sample changers

The commands in this section can be used with the sample changers, as follows:

	PW1500/00 - 6 position	PW1500/10 - 72 position
LTU	Y	Y
UTU	Y	Y
STY	N*	Y
MTY	Y	Y
FRT	Y+	N
SRT	Y+	N
ASC	Y	Y
RCS	N	Y
PTY	Y	Y

* The command is not inhibited, but it is not useful

\+ These commands can only be used with the reference tray option PW1505/00

▲ LTU i — Load sample from the changer into turret position i, where i = 1 to 4.

▲ UTU i — Unload sample from turret position i to the changer, where i = 1 to 4.

▲ STY i — Search for tray number i, where i = 1 to 165 (coded on tray program card). The changer will search until position 1 of the selected tray number i is in position ready to be loaded into the spectrometer.

▲ MTY i — Move the tray to bring the tray position i ready for loading, where i = 1 to 6.

▲ FRT — Fetch the tray of reference samples, stored in the PW1500/00 six-position changer, with reference tray option PW 1505/00.
Refer to paragraph 3.1.

▲ SRT — Store the samples from the turret back into the reference tray (PW1500/00 with reference tray option PW1505/00).

ASC i (j) — Automatic sample changer to be used for the measurement of samples up to, and including, tray i, where i = 1 to 165. The optional argument j is an identification number from 0 to 999, which is raised by 1 for each new sample loading.

RCS i	Recycle sample changer measurements i times. i = as RCM command.
PTY i	Programmed tray i, where i = 1 to 165,can have a separate measurement program and sample identification for each sample.

Stop commands

/	Stop measurement program (or other action) immediately after slash **and** carriage return given.
/S	Stop the scaler/timer operation and print the results. If a further measurement is programmed, this will start after the printout of the results.
/M	Stop after the completion of the measuring program of the samples. Used to interrupt a recycling program, or to interrupt a measurement routine using the automatic sample changer. The original recycling command is not reset.
/T	Stop after the complete measurement of samples in a tray in the loading position of the automatic sample changer. The next start measurement command will commence measurement of the samples in the next tray.

Computer command

AUT	Return to computer dialog, when a computer is connected.

Error messages

The following error messages are generated during programming or measurement. Examples of some of these messages are included in the description of programming and analysis, where appropriate.
Note that error messages generated by the microprocessor software are prefixed with two asterisks (**), while error messages generated by the computer software (paragraph 2) will be prefixed with three asterisks.

OUTPUT	MEANING
ERROR COMMAND NOT AVAILABLE	Incorrect command given, not in microprocessor software.
INVALID ARGUMENT	Argument not correct or incomplete. Repeat command with proper argument.
INVALID, CORRECT VALUE (S)	Incorrect value entered during list assembly, and will require the correct value to be input before the list assembly can proceed.
MP . . ** NOT IN MEMORY	Requested measurement parameters list not assembled and stored in the memory, e.g. when requested by SMX.
NOT IN MEMORY	Requested channel set, MP list or job list has not been assembled.
NO MORE SPACE AVAILABLE	The maximum (63) channel sets have already been assembled in the parameter bank.
LIST OVERFLOW	MP list or job list is more than 255 bytes, refer to paragraph 1.3.4.
ERROR JOB	Job started from sample changer card contains commands not allowed (▲ in chapter 2.2.)

MEMORY OVERFLOW	Too many MP lists and job lists in the parameter bank - see paragraph 1.3.4.
GENERATOR OFF	Given when a program or command requests generator settings (not manual) but the H.T. is switched off.
NOT ALLOWED IN POSITION	Output if LDM2 is given in continuous mode (CMD)
ERROR MONITOR LOADED IN POSITION	Attempt to load an unknown sample into a turret position that contains a monitor. Either unload the monitor first with the ULM command, or load the unknown into another turret position.
ERROR NO MONITOR IN POSITION	Monitor sample has not been loaded (by LDM command) in the MOPS turret position.
ERROR MONITOR	Monitor not in turret or sample changer, or M-bit is selected for absolute measurement program.
NO BUF RAT	The measurement program selected by a SMM command is for absolute or direct ratio measurement, i.e. not buffer ratio.
ERROR BATTERY, PARAMETER BANK CLEARED	Data not in memory, either due to the removal of the RAM card, or the battery supply to the card being low when mains power is disconnected.
ERROR > 80 CHAR	Any line of operator typed characters (command, arguments, spaces, identification, etc.) must be less than 80 before carriage return is given.
ERROR WRONG CHAR AFTER / :=	Character given in a stop command is not correct (can be S, M T or C).
ERROR PRINTER 2	Output to a second device is requested (SOT Y) but connection to device is not present. Output is not inhibited (output will only appear at the main terminal).
ERROR xx	Error detected and xx is a hexa-decimal code - refer to the Service Manual.
ERROR VACUUM	Hardware indicates a vacuum fault condition. Operation is not inhibited.
ERROR ANGLE ERROR COLLIMATOR ERROR FILTER ERROR MASK ERROR CRYSTAL ERROR CAP ERROR PLUNGER ERROR TURRET ERROR DETECTOR GAS ERROR MEDIUM	Spectrometer hardware gives a fault indication, or non-compliance with a command, and operation is inhibited. Refer to the Service Manual for futher details.
ERROR FRAMING ERROR OVERRUN ERROR PARITY	Error indication due to peripheral connection - refer to the Service Manual for further details.
ERROR PROM x ————	Check of PROMS and RAMS when system switched on, or reset, shows an error - refer to Service Manual.
ERROR RAM	
ERROR SAMPLE CHANGER xx	Operation error when the sample changer is used, where xx is a code to define the error. A listing of the errors is given in paragraphs 3.1./3.2. Note that an error message will also be given if a sample changer is not connected, but a changer command is typed.

PW1400 SYSTEM COMMANDS LIST

For general information a complete listing of commands, in alphabetical order, is shown below.
The list indicates whether the commands can be given in the MAN (microprocessor) mode, or the AUT (computer) mode, (or both). If the meaning column explanation is not clear a reference to a disc module is given in brackets.

Computer commands (AUT) marked with a P are not used in the DEC PDP 11 software

Used in MAN	Used in AUT	Command	Meaning
●	●	/	Emergency stop-abort measurement
●	●	/S	Stop the counter/timer
●	●	/M	Stop after measurement program completed
●	●	/T	Stop after measurement of sample in changer tray
	●	ACD	Assemble concentration data
●	●	ACH	Assemble/change channel set
	●	ACP	Assemble/change calculation parameters
	●	ADC	Add a channel (update)
	●	ADF	Add a file (update)
	●	ADS	Add a sample (update)
●	●	AJB	Assemble a job list
●		ALL	Assemble a limits list
	●	ALP	Assemble/ change a link program list
	●	AMB	Assemble/ change monitor buffer list
	●	AML	Assemble/ change a moduli list
●	●	AMP	Assemble/ change a measurement parameters list
	●	AMS	Assemble/ change a moduli set
	●	ANM	Assemble/ change the long names listing
	●	ARC	Assemble/ change a countrate correction set.
●	●	ASC	Automatic sample changer measurement.
	●	ASP	Assemble/ change the system parameters
●		AUT	Switch to automatic mode - computer control
●	●	BMD	Batch mode measurement
	●	CAL	Calculate element alpha (regression)
●	●	CAN	Calibrate goniometer angle
	●	CBT	Calculate element beta (regression)
	●	CCD	Correct concentration data (regression)
	●	CEB	Change equivalent background (regression)
	●	CHC	Change concentration data (update)
	●	CHI	Change intensity data (update)
	●	CID	Correct intensity data (regression)
	●	CLF	Close the file (update)
●	●	CMD	Continuous mode measurement
●		COL	Collimator selection
●		COM	Communicate with second terminal

MAN	AUT	Command	Meaning
●	●	CPB	Clear parameter bank data
	●P	CPD	Copy disc data
	●P	CPF	Copy a file
	●	CST	Calculate statistics (update)
●		CTS	Continuous scan with goniometer
	●	DCP	Delete calculation parameters list
●		DET	Select detector
●	●	DJB	Delete job list
	●	DLC	Delete channel from file (update)
	●P	DLF	Delete file data (update)
	●	DLL	Delete limits list
	●	DLP	Delete link program list
	●	DLS	Delete sample from file (update)
	●	DMB	Delete a monitor buffer list
	●	DML	Delete a moduli list
●	●	DMP	Delete a measurment parameter list
	●	DMS	Delete a moduli set.
●	●	DPB	Dump the parameter bank data
	●	DRC	Delete a countrate correction set
	●	DSA	Delete a sample (s) from regression calculation
●	●	EJB	End of a job list assembly
●		EJB	End of a job list assembly
	●	END	End the X14 software program operation
	●	FAL	Fix the alpha in the regression calculation
	●	FBT	Fix the beta in the regression calculation
●		FLT	Select beam filter
●	●	FRT	Fetch the reference tray
	●	FTM	Finish transmission to second terminal
	●P	IND	Initiate a flexible disc (update)
	●	ISA	Include sample again in the regression calculation
●	●	KVM	Select kV and mA valueson generator
	●	LDB	Load databank into the computer memory from the flexible disc
●	●	LDM	Load a monitor sample into a turret position
●	●	LTU	Load a turret position with a sample from the changer
●		LWL	Set lower level value of pulse height discriminator
	●	MAN	Change to manual (microprocessor) mode of operation
●	●	MPY	Multiply the PC/PT settings (in MP list)
●		MSK	Select collimator mask position
●	●	MTY	Move changer tray to the loading position
	●	NDD	No data to disc (reset of WDD- analysis)
	●	NPI	No printing of gross intensities (reset of PIN)
	●	NRE	Next regression element for analysis

MAN	AUT	Command	Meaning
●		NRL	Number of lines on VDU
	●P	ONL	On-Line spectrometer operation
	●	OPF	Open file on floppy disc (update)
●		ORD	Select order of reflection
	●	PCD	Print concentration data (update)
●	●	PCH	Print channel parameters
	●	PCI	Print concentration and intensity data (update)
	●	PCP	Print calculation parameters list
●		PCS	Preset counts setting
●	●	PHD	Pulse height distribution measurement
	●	PID	Print intensity data (update)
	●	PIN	Print intensity results (analysis)
	●	PJF	Print job file (job results) from file opened with OPF (update)
	●	PLL	Print limits list
	●	PLP	Print link program list
	●	PLS	Plot a step scan spectrum
	●	PMB	Print monitor buffer list
	●	PML	Print moduli list
	●	PMM	Print memory map of the databank
●	●	PMP	Print measurement parameters list
	●	PMS	Print moduli set
	●	PNM	Print long names listing
●	●	PPB	Print parameter bank details
	●	PRC	Print countrate correction set
	●P	PRD	Print the directory data of disc
	●	PRL	Print a list of the calculated concentrations (regression)
	●	PSI	Print sample identification (update)
	●	PSP	Print system parameters (assembly)
●		PTC	Preset time and count setting
●		PTS	Preset time setting
●	●	PTY	Program tray conditions
●	●	PWR	Maximum power and kV generator settings defined
	●	RCF	Reset correction factor (regression)
●	●	RCJ	Recycle the job measurement program
●	●	RCM	Recycle measurement program
●	●	RCS	Recycle sample changer measurements
●	●	RES	Reset MPY, RCM, RCJ, RCS and ASC commands
●		RMS	Ratemeter full-scale range setting
●	●	RPB	Read parameter bank
	●	RTM	Request transmission to second terminal (analysis)
	●	SAR	Start automatic recalibration (analysis)

MAN	AUT	Command	Meaning
●		SCH	Set the channel parameters
●		SCT	Start counter/timer
●	●	SJB	Start job measurement
●		SLF	Slew goniometer with fast speed
●	●	SLP	Sample turret position to loading position
●		SLS	Slew goniometer with slow speed
	●	SMA	Start measurement of apparent concentrations (analysis)
●	●	SMM	Start monitor measurement
●	●	SMP	Sample turret position to measuring position
	●	SMR	Start manual recalibration (analysis)
●	●	SMX	Start measuring unknown samples
●		SOT	Transmit to second output terminal
●	●	SPN	Sample spinner operation
	●	SPR	Start prepare regression intensities (analysis)
	●	SRA	Start regression analysis (regression)
	●	SRI	Start regression input (regression)
	●	SRP	Start regression and print results (regression)
	●	SRR	Save regression results (regression)
●	●	SRT	Store reference tray
●		SSM	Single step mode for goniometer
	●	SSR	Start semi-automatic recalibration (analysis)
	●	STM	Start transmission to second terminal (analysis)
●		STS	Step scan with goniometer
●	●	STY	Search changer tray
●	●	ULM	Unload monitor sample from turret
●		UPL	Set upper level value of the pulse height discriminator
●	●	UTU	Unload sample from turret to the sample changer tray
	●	WDB	Write databank contents to disc (assembly)
	●	WDD	Write measurement data to disc (analysis)
●		XTL	Select crystal

1.3. PREPARING THE MEASUREMENT PROGRAM

The measurement of samples will require the assembly of sets of channel parameters, one set for each element line in the analysis. Also required will be one or more lists of measurement parameters, called MP lists. In addition job lists can be assembled to include MP lists, goniometer scans, etc., as described in paragraph 1.3.3.

Important. When the equipment is first switched on the H.T. generator maximum power and kV value must be defined, using the PWR command, otherwise the channel sets cannot be completed - see figure 1.3A.

Before commencing the assembly of sets of parameters required for analysis of a new series of samples, it is an advantage to check the contents of the parameter bank using the PPB command. This command will include details of the free space in the memory, refer to paragraph 1.3.4. Use the print commands (PCH and PMP) to obtain detailed information on the channel sets and MP lists already assembled, but note that a readout of existing job lists is not possible.

1.3.1. Assembling a channel set.

A new channel set can be assembled by the command ACH, or an existing set can be changed using ACH xxi. The channel sets are stored in the memory in the order in which they are assembled, and they cannot be deleted except by overwriting with another set of channel parameters, or unless the whole parameter bank is cleared. The set of channel parameters includes all spectrometer system settings except the operation of the spinner (SPN command), the selection of the collimator mask (MSK i command), and the preset time and/or counts which will be defined in the measurement program (MP list).

Up to 63 channel sets can be assembled, and paragraph 1.3.4. gives information on the organisation of the memory space in the parameter bank.

If the ACH command is given, the first or next free channel space will be allocated in the parameter bank. If ACH xxi is given the parameter bank is searched for the required channel information. After assembly a print of all (PCH) channels, or a particular (PCH xxi) channel can be obtained. Note that the arguments xxi can be made up of one or two letters (normally the element symbol), and an optional number 1 to 3 to indicate channel parameters which differ from the standard element, e.g. in case of line overlap.

Dialog with the microprocessor is as follows, and is illustrated in figure 1.3A.

NAME : = no check against periodic chart	One or two letters to identify the element, and an optional number 1 to 3.
LINE : =	KA, KB, LA, LB, LG or MA to identify the line of the spectrum.
FLT : = none in our machine	Beam filter in (Y = yes) or out (N = no).
COL : =	Collimator fine (F = 150 μm spacing), or coarse (C = 550μm spacing).
DET : =	Detector flow (F), or scintillation (S) or both (FS).
XTL : =	Select crystal changer position 1 to 6 (keep a note of the crystal type fitted in each changer position). The changer drive is bidirectional and rotation to a new position is by the shortest route.
ORD : =	Order of reflection, first (1) or second (2).
UPL : =	Percentage value of upper level setting of the window (0 to 99 in 1% steps). If the zero value is chosen the upper level setting is infinity.
LWL : =	Lower level setting (0 to 99 in 1% steps). If the lower level value is higher than the upper level the window is set at zero and detector pulses will not be counted.

Keyboard lock in upper case

KV, MA : = H.T. generator output setting of 25 to 100 (kV) in 5 kV steps, and of 10 to 80 (mA) in 5 mA steps. A zero value is acceptable in which case the manual setting of the generator controls is made when the channel set is selected during analysis. An error message will be generated if the PWR command values are exceeded or the command is not active (is zero) during assembly, also if a program selects output values but the high-voltage is not switched on.

ANGLE : = Goniometer 2θ angle setting, 0 to 147.000 in 0.005^{o} steps.

+ OFFS : =
– OFFS : = Offset angle from the goniometer ANGLE = setting, of 0 to 5.10 ($^{o}2\theta$) in 0.02 steps. In the MP list assembly the channel can be shown as xxi+ and/or xxi–, and the goniometer goes to the xxi angle ± the offset angle.

A carriage return is given as input if the parameter presented in the software dialog does not require change. If a channel set is being changed, the list assembly can be terminated by a / (slash) after the required changes have been input.

```
C=PWR 2.5 60
```
Generator output limited to 2 1/2 kW and 60 kV

```
C=ACH                          Assemble a (new) channel set
NAME:          :=CU            Name of set is copper — to be used in MP list assembly, etc.
LINE:   KA  :=                 Kα line (Kβ, Lα, Lβ, Lγ and Mα also permitted.
FLT  :  NO  :=                 Filter: no or yes, c.r. given so no filter selected.
COL  :  F   :=                 Collimator: fine (F) or coarse (C)
DET  :  FS  :=F                Detector: flow (F), scintillation (S), or both (FS)
XTL  :  1   :=                 Crystal: position 1 (in this case 1 = LiF 200)
ORD  :  1   :=                 Order of reflection: 1 or 2
UPL  :    0 :=75               Upper limit of window: 0 to 99%
LWL  :    0 :=25               Lower limit of window: 0 to 99%
KV,MA:      0     0 :=50 60    Generator setting: In this case more than 2,5kW (PWR command), therefore
                               an error message is generated. Also error if PWR not given in start up.
** INVALID, CORRECT VALUE(S) =50 50
ANGLE:        .000 :=45030     Goniometer angle setting for element line: 0 to 147.000° 2θ,
                               therefore error message is generated.
** INVALID, CORRECT VALUE(S) =45.030
+OFFS:        .00  :=1         Angle offset values: 0 to 5.10 (°2θ), refer to paragraph 1.3.2. for use.
-OFFS:        .00  :=
C=PWR 3 100
```

```
C=ACH
NAME:          :=SI
LINE:   KA  :=
FLT  :  NO  :=
COL  :  F   :=C
DET  :  FS  :=F
XTL  :  1   :=4
ORD  :  1   :=
UPL  :    0 :=80
LWL  :    0 :=20
KV,MA:      0     0 :=50 60
ANGLE:        .000 :=109.21
+OFFS:        .00  :=2
-OFFS:        .00  :=2
C=PWR 3 100
```
Assembly of a second channel set (for Si).

Figure 1.3.A Assembly of channel sets (continued on next page).

```
C=ACH SI
NAME:   SI     :=
LINE:   KA     :=
FLT  :  NO     :=
COL  :  C      :=
DET  :  F      :=
XTL  :  4      :=
ORD  :  1      :=
UPL  :  80     :=
LWL  :  20     :=
KV,MA:    50   60  :=50  30
ANGLE:   109.210  :=
+OFFS:     2.00   :=
-OFFS:     2.00   :=
C=
```

Channel list for silicon is already in the memory, but must be changed.

No change, so give c.r.

New values of kV and mA input

Figure 1.3.A. Assembly of channel sets. (also see previous page)

The following table (figure 1.3B) shows sets of channel parameters covering most element lines. These are typical only, and may not be optimised for a particular requirement. Values will depend on the type of sample measurement requirements, etc.

The tables are based on the use of a chromium tube, and the crystal changer has a LiF200 crystal in position 1, a PE in 2, a TIAP in 3, and a Ge in position 4.
The kV and mA values apply when a 100 kV generator is connected, and for a 60 kV generator the values should be 50/60 from element F to Ni and Cs to Hf, and 60/50 from Cu to I and Ta to U, or as required.

```
C=PCH
ELEMENT FLT COL DET XTL ORD UPL LWL   KV  MA    ANGLE  +OFFS  -OFFS

F       KA  NO  C   F   3   1   80  20  50  60  90.710   2.00   2.00
F2      KA  NO  F   F   3   1   65  30  50  60  90.710    .00   2.00
NA      KA  NO  C   F   3   1   80  20  50  60  55.100   3.00   2.00
MG      KA  NO  C   F   3   1   80  20  50  60  45.170   2.00   2.00
MG2     KA  NO  F   F   3   1   65  30  50  60  45.170    .00   2.00

AL      KA  NO  C   F   2   1   75  25  50  60 145.130   2.00   2.00
SI      KA  NO  C   F   2   1   75  25  50  60 109.210   2.00   2.00
P       KA  NO  C   F   4   1   75  25  50  60 141.040   2.00   2.00
P2      KA  NO  F   F   4   1   75  25  50  60 141.040   3.00    .00
S       KA  NO  C   F   4   1   75  25  50  60 110.690   2.00   2.00

S2      KA  NO  F   F   4   1   75  25  50  60 110.690    .00   2.00
CL      KA  NO  C   F   4   1   75  25  50  60  92.760   2.00   2.00
K       KA  NO  C   F   1   1   75  25  50  60 136.690   2.00   2.00
CA      KA  NO  C   F   1   1   75  25  50  60 113.090   2.00   2.00
CA2     KB  NO  F   F   1   1   75  25  50  60 100.230   2.00   2.00

TI      KA  NO  F   F   1   1   75  27  50  60  86.140    .00   2.00
V       KA  NO  F   F   1   1   75  30  50  60  76.930    .00   2.00
CR      KA  YE  F   F   1   1   75  15  50  60  69.360   2.00    .00
MN      KA  YE  F   F   1   1   75  17  50  60  62.970   2.00    .00
FE      KA  NO  F   F   1   1   75  20  50  60  57.520   2.00    .00
```

Continued from previous page

CO	KA	NO	F	F	1	1	75	20	50	60	52.800	2.00	.00
NI	KA	NO	F	F	1	1	75	22	50	60	48.670	1.00	.00
CU	KA	NO	F	F	1	1	75	22	60	50	45.030	1.00	.00
CU2	KB	NO	F	F	1	1	75	24	60	50	40.450	.00	1.00
ZN	KA	NO	F	F	1	1	75	24	60	50	41.800	1.00	.00
GA	KA	NO	F	FS	1	1	75	25	60	50	38.920	1.00	1.00
GE	KA	NO	F	FS	1	1	70	25	60	50	36.330	2.00	1.00
AS	KA	NO	F	FS	1	1	70	25	75	40	34.000	.00	1.00
SE	KA	NO	F	FS	1	1	70	25	75	40	31.890	1.00	1.00
BR	KA	NO	F	FS	1	1	75	25	75	40	29.970	1.00	1.00
RB	KA	NO	F	FS	1	1	75	25	75	40	26.620	1.00	.00
SR	KA	NO	F	FS	1	1	75	25	75	40	25.150	1.00	1.00
Y	KA	NO	F	FS	1	1	75	25	75	40	23.800	1.00	1.00
ZR	KA	NO	F	FS	1	1	75	25	75	40	22.550	.80	.80
NB	KA	NO	F	FS	1	1	75	25	75	40	21.400	1.60	.80
MO	KA	NO	F	FS	1	1	75	25	100	30	20.330	1.50	1.50
RU	KA	NO	F	FS	1	1	75	25	100	30	18.420	1.00	1.00
RH	KA	NO	F	FS	1	1	75	25	100	30	17.560	.00	1.00
PD	KA	NO	F	FS	1	1	75	25	100	30	16.760	1.70	1.70
AG	KA	NO	F	FS	1	1	75	25	100	30	16.010	1.00	1.00
CD	KA	NO	F	FS	1	1	75	25	100	30	15.310	1.00	1.00
IN	KA	NO	F	FS	1	1	75	25	100	30	14.660	1.00	1.00
SN	KA	NO	F	FS	1	1	75	25	100	30	14.040	1.00	1.00
SB	KA	NO	F	S	1	1	75	25	100	30	13.460	1.00	1.00
TE	KA	NO	F	S	1	1	75	25	100	30	12.910	1.00	1.00
I	KA	NO	F	S	1	1	75	25	100	30	12.400	.70	.70
CS	LA	NO	F	F	1	1	75	25	50	60	91.830	2.00	2.00
BA	LA	NO	F	F	1	1	75	27	50	60	87.170	2.00	.00
LA	LA	NO	F	F	1	1	75	28	50	60	82.910	2.00	2.00
CE	LA	NO	F	F	1	1	75	30	50	60	79.010	2.00	2.00
HF	LA	NO	F	F	1	1	75	22	50	60	45.880	1.50	1.50
TA	LA	NO	F	F	1	1	75	22	60	50	44.420	1.50	1.50
W	LA	NO	F	F	1	1	75	22	60	50	43.020	1.00	2.00
RE	LA	NO	F	F	1	1	75	24	60	50	41.690	1.00	1.00
OS	LA	NO	F	FS	1	1	75	25	60	50	40.420	1.00	1.00
IR	LA	NO	F	FS	1	1	75	25	60	50	39.220	1.00	1.00
PT	LA	NO	F	FS	1	1	70	25	60	50	38.060	1.00	.00
AU	LA	NO	F	FS	1	1	70	25	60	50	36.960	2.00	2.00
HG	LA	NO	F	FS	1	1	70	25	75	40	35.910	.00	.00
PB	LA	NO	F	FS	1	1	70	25	75	40	33.930	1.50	1.20
BI	LA	NO	F	FS	1	1	70	25	75	40	33.010	1.00	1.00
RA	LA	NO	F	FS	1	1	75	25	100	30	28.900	1.20	1.20
U	LA	NO	F	FS	1	1	75	25	100	30	24.140	1.50	1.50

C=

Figure 1.3.B. Table of typical channel parameters

1.3.2. Assembling a measurement parameters list.

The measurement parameters (MP) list will contain the parameters necessary for the measurement of samples (unknown and monitor). The list must contain the channel name, preset time and/or preset count of all element lines to be measured. In the event of no input (carriage return), default values will be stored as shown. Paragraph 1.4 gives further details of the assembly of an MP list, depending on whether the measurement is to be absolute, direct ratio or buffer ratio.

To assemble or change an MP list, type AMP followed by a number 1 to 63. The assembled list will be stored in the parameter bank, and a selected MP list contents will be printed by the command PMP 1 to 63. The numbers (1 to 63) of all the MP lists which are stored in the parameter bank are listed in the readout from the PPB M or PPB commands.

Dialog with the computer is as follows, and is illustrated in figures 1.3C and 1.3D.

MASK : 1 : =	Select collimator mask 1 or 2, refer to paragraph 1.6.3.
ABS : YE : =	Absolute measurement (give c.r.) or ratio measurement (give N or NO)

The following dialog (BRAT, MOPS and MOMPY) is output for ratio measurement, i.e. if ABS = YE go to CHAN/PT/PC.

BRAT : = NO : =	Buffer ratio measurement selection, give c.r. or NO for direct ratio, or YE for buffered ratio. Refer to paragraph 1.4.
MOPS : = 1 : =	Monitor sample position in the turret, use positions 1, 2 or 3 in batch mode, or positions 1 or 3 in continuous mode (BMD or CMD given before sample measurement).
MOMPY : = 1 : =	Monitor sample measurement multiplication factor, set to 1, 2, 4, 10, 20 or 40. The preset time (PT) and preset counts (PC) set for the channel elements below are multiplied by this factor when the monitor sample is measured.
CHAN PT PC	For each element channel required in the measurement program, the preset time and/or count is selected as follows:
CHAN	Give the element channel name as specified in the channel set (ACH) assembly (NAME =), and if required, a + or — if measurement of backgrounds is required at the 2θ angle + or — the offset angle.
PT	Preset time for the measurement: 0, 2, 4, 6, 8 ,10, 16, 20, 40, 50, 80, 100, 200, 400, 800 or 999 (seconds). Default value is 0 (infinity).
PC	Preset count to stop the measurement from 1E4 to 5E7, where the first digit can be 1, 2 or 5. E indicates Exponential, and the last digit can be 4 to 7, i.e. from 10 000 to 50 000 000, Default value is zero (infinity).

If values are entered for PT and PC, the measurement will stop when the first of the values is reached. If either PT or PC is set to zero (or a value is not entered), if the PT or PC counter reached its maximum value before the preset stop value, the counter will reset and continue counting. In this case an overflow indication is not generated.

Following a start measurement command, the elements will be measured according to the order of assembly in the MP list, and if more than one MP list is used in the measurement they will be selected in the order as input by the start measurement command. To reduce the time required for mechanical movement of the spectrometer, try to assemble the MP list in the following order of element channels:

- heaviest elements first
- group all channels using the same crystal
- select lines in increasing order of goniometer angle, for example, a - offset angle before the peak angle.

```
                                        C=PMP 10        Print MP10

C=AMP 10        Assemble MP10           MP 10

MASK :  1 :=2                           MASK :  2       Collimator mask 2 selected
ABS  : YE :=                            ABS  : YE       Absolute measurement

CHAN    PT    PC                        CHAN    PT    PC
          0   0E0 :=FE 10               FE      10    0E0   Preset time values only input, for element and
          0   0E0 :=CA2 20              CA2     20    0E0   background channels, etc.
          0   0E0 :=K 4                 K        4    0E0
          0   0E0 :=S 10                S       10    0E0   Sulphur peak
          0   0E0 :=S+ 10               S+      10    0E0   Sulphur peak plus offset (given in ACH S list)
          0   0E0 :=SI 20               SI      20    0E0
          0   0E0 :=AL 20               AL      20    0E0
          0   0E0 :=MG2- 20            MG2-    20    0E0   MG 2 peak minus offset
          0   0E0 :=MG2 40             MG2     40    0E0
          0   0E0 :=NA 40              NA      40    0E0
          0   0E0 :=NA+ 20             NA+     20    0E0
          0   0E0 :=                   C=
                 /
C=
```

Figure 1.3C Assemble/print measurement parameters list

MP 10 is a program for the measurement of cement samples. In this program the CaKβ line is chosen for measurement as the Kα line is too intense. For the measurement of the magnesium channel, Mg2 is chosen to minimise higher order interference from calcium. Backgrounds are measured for sulphur, magnesium and sodium.

```
C=AMP 41

MASK :  1 :=
ABS  : YE :=N      Not absolute, i.e. ratio measurement
BRAT : NO :=       Not buffer ratio, i.e. direct ratio
MOPS :  1 :=       Monitor sample to be in turret position 1
MOMPY:  1 :=       Monitor multiply factor = 1, i.e. PT and PC as for unknowns

CHAN    PT    PC
          0   0E0 :=SN 10
          0   0E0 :=PB 10
          0   0E0 :=ZN 0 1E7   }  Preset time is zero (infinity) and preset count will stop
          0   0E0 :=CU2 0 1E7  }  measurement (10^7 counts). In this case PT = 0 means that
          0   0E0 :=NI 4          sample measurement will show ratio values for Zn and CuK$\beta$.
          0   0E0 :=FE 4
          0   0E0 :=MN 10
          0   0E0 :=AL 10
          0   0E0 :=
                 /
C=
```

Figure 1.3D Assembly of a direct ratio MP list

MP41 is a measurement program for brass samples. High precision is required for copper and zinc. These two elements are measured in direct ratio, the other elements are measured in absolute mode. For copper the Kβ line is chosen as the Kα line is too intense.

1.3.3. Assembling a job list

Up to 63 job lists can be assembled using the command AJB. Note that a print of the job listing is not possible, therefore, ensure that a hard copy readout is saved from the original assembly. Also a job list cannot be changed, it can only be deleted and re-assembled.

The commands that can be used in a job list are shown in the command list marked with a solid square ■ and a solid triangle ▲. The selection of a job list measurement can be made from a typed command, or from the sample tray identification card when the sample changer is installed. With sample changer selection it is not possible to use the SMM command in a job list, or commands associated with the sample changer operation.

Using any combination of the commands, marked as above, it is possible to perform a wide variety of measurements, such as using a separate measurement program for each sample loaded in a different turret position, making step and/or continuous scans over several peaks with readout to a chart recorder and/or printer, etc. Examples of job assembly are shown in 1.3E and 1.3F, and the measurement and results are described in paragraph 1.4.7.

```
C=AJB 33          Assemble job list 33
                  Job routine now uses J =
J=SMX 13          Start measuring unknown samples using MP list 13
SAM.POS :=1       Sample loaded in turret position 1
J=SMX 14
SAM.POS :=2
J=SMX 15          Separate measuring programs used for each turret sample position
SAM.POS :=3
J=SMX 16
SAM.POS :=4
J=EJB             End of job listing. Revert to normal C = dialog

C=
```

Figure 1.3E Job list for separate measuring program per turret position

C=AJB 35	Assemble job list 35
J=SCH FE	Set spectrometer to Fe channel parameters
J=SLF 56	Goniometer slew fast to 56° 2θ
J=RMS 1E5	Set ratemeter range to 100 000 counts (full scale)
J=CTS 59 2	Continuous scan to 59° (from 56°) 2θ, with speed 2° 2θ/minute (Fe peak)
J=SLF 61	Slew fast to 61° 2θ
J=FLT Y	Set beam filter in (to remove interfering tube lines)
J=CTS 64 2	Continuous scan to 64° 2θ (Mn peak)
J=SLF 68 J=CTS 71 2	Scan from 68 to 71°2θ (Cr peak, filter in)
J=SLF 76 J=FLT N J=CTS 78 2	Scan from 76 to 78 2θ, (V peak, filter out)
J=SLF 85 J=RMS 2E5 J=CTS 87 2	Scan from 85 to 87°2θ, with ratemeter scale = 2 x 10^5 (Ti peak)
J=SLF 111 J=COL C J=RMS 1E5 J=CTS 115 2	Scan from 111 to 115° 2θ, with coarse collimator and ratemeter scale = 10^5. (Ca peak)
J=SLF 135 J=CTS 138 2	Scan from 135 to 138° 2θ (K peak)
J=SCH K J=PTS 10 J=SCT	Precise measurement of the K peak at 137.69° 2θ, using the channel K parameters, and counting for 10 seconds.
J=EJB	End of job listing
C=	C = dialog

Figure 1.3F Job list for peak scanning (refer to paragraph 1.4.7).

1.3.4. Parameter bank operation

The parameter bank is the part of the memory which contains:
- a fixed space of 630 words for the assembly of **63** sets of channel parameters (ACH command)
- space for the assembly of up to 63 measurement parameter lists (AMP command)
- the same space for the assembly of up to 63 job lists (AJB command).

The MP lists and job lists can be variable in length, therefore, the 63 lists maximum above only refers to the number which is allocated to the list, i.e. MP64 or JB64 are not allowed. The initial space available for these list is not less than 800 words, and space will be taken as follows:
- MP list = 3 words plus 2 words per channel
- JB list = 3 words plus 3 words (average) per command.

If any list is longer than 255 bytes the error message "LIST OVERFLOW" is printed.

When the PPB command is given, the readout of the parameter bank details will show the free space available for the assembly of new MP and JB lists.

The data stored in the parameter bank (RAM card) is protected in the event of mains failure or disconnection, by a battery fitted on the bus interface card. A fully charged battery will maintain the data for at least 500 hours. **Parameter bank data will be lost if the RAM card is pulled out from its connector.**
Other instrument condition commands, principally PWR (maximum generator power and kV), are also stored in the RAM card, but not in the parameter bank. Therefore, these commands are not affected when the parameter bank is cleared (CPB command), or new data is read in (RPB command).

The main parameter bank details are printed from the PPB command as follows:
- PPB (no arguments); a listing of channel names, numbers of MP lists and numbers of job lists already assembled, and the free space available (about 800 words with an empty parameter bank).
- PPB C; channel names only
- PPB M; numbers of measurement parameter lists only
- PPB J; numbers of job lists only
- PPB F; print free space only.

A typical readout of the parameter bank details is shown in figure 1.3.G.

A detailed readout of the stored data in the parameter bank is obtained as follows:
- PCH ; print **all** channel parameters
- PCHxxi ; print parameters of channel xxi only
- PMP i ; print parameters of MP list i.

The readout from these commands are shown in various figures in paragraph 1.

A readout of the job list is not given, therefore, details of the various job list assemblies must be kept for future reference.

```
C=PPB      Print parameter bank
F    F2   NA   MG   MG2  AL   SI   P    P2   S    S2   CL   K    CA   CA2
TI   V    CR   MN   FE   CO   NI   CU   CU2  ZN   GA   GE   AS   SE   BR
RB   SR   Y    ZR   NB   MO   RU   RH   PD   AG   CD   IN   SN   SB   TE
I    CS   BA   LA   CE   HF   TA   W    RE   OS   IR   PT   AU   HG   PB
BI   RA   U

MP 10
MP 12
MP 17
MP 40
MP 41
MP 42
JB 21
JB 22
JB 23
JB 24
JB 25
JB 32
JB 33
JB 34
JB 35
JB 39
FREE SPACE :   493 WORDS
C=


C=PPB M    Print MP listing in parameter bank
MP 10
MP 12
MP 17
MP 40
MP 41
MP 42
FREE SPACE :   493 WORDS
C=
```

Figure 1.3G Print parameter bank readout

Three commands are associated with the parameter bank operation:
- DPB ; dump parameter bank data
- RPB ; read parameter bank data into the microprocessor (RAM)
- CPB ; clear parameter bank (all data to zero).

The information in the parameter bank is in hexa-decimal format, which can be readout to a paper tape punch (or similar) using the DPB command. The data is still retained in the parameter bank. A typical **printer** readout is shown in figure 1.3H.

```
C=DPB          Dump parameter bank (hexa-decimal readout)
$$$$$
0600455014582366F6464460044461458236F00640E01455014581586966400D07455014
5B11A564644D07444614581 1A5006401 0C2550145B38B1646413092550145B2AA96464
1000655014583718646450006450145B37189600130065501 45B2B3D6464530064501 4
5B2B3D0064030C6550145B243C64640B000550195B3565646403010550195B2C2D6464
4321045019582727646414090450195B21A6006416000450 1E5B1E0D00640312065011
5B1B1864000D0E0650145B18996400060504 4B145B16786400030F044B145B14A06400
0E09044B195B1303320003150 44B19791197320043350 44B19790FCD00321A0E044B19
791054320007010 04B14790F34323207050046147 90E31643201130046147 90D480032
1305004614790C753232021200501479 0BB5323212020050147 90A6632001312005014
7909D3323219000050147 9094C32321A1200501479 08CF28280E0200501479085C5028
0D0F0050147907F14B4B1215005014790732323212080050147906DC00321004005014
79068C555501070050147906413232030400501479 05FB3232090E005014790 5BA3232
130E005014790 57C3232130208501479054232321405085014790 50B3232090008501 4
7904D8232303530450195B23DF6464024104501 95B220D64000C4104501 95B20636464
0345045 01E5B1EDD6464084604 4B195B11EC4B4B1441044B1979115A4B4B1740044B19
7910CE3264124504 4B19791049323 20F5300501479 0FCA3232095200501479 0F523232
1054004614790EDE3200015500461479 0E706464084700461479 0E0700001042004614
790D414B3C0249004614790CE5323212410050147 90B4A3C3C1540005014790A364B4B
0000000000000000000000000000000000BC010A1905145 00F700D200A504A500770
0670857005800380437 00C3508195059501750575016501450545013705350127090 20
1020305 00F708D200D208A500A5008500770472006700570837003801109D916501407
12542813C12B503C5019701770162014201350065029138 02B503C50190A180A162014
20135006502A13812B503C5019BA18BA1620142013500650551 20A1502EC1346181 58B
024C1D46DC1E0056130A1302D41746001 90E8B025424468025005 71F0A1903640008 02
CC1008100254100802CC1008500254100802CC1008005814 0A2403640013 5B0813790 8
13A70813F5080059250A0512500230116 6C012124602301166C012124102301166C012
111E02301166C01200600C1536D6371A2800003800611399 0D0000198E0000190F8000
191000800062420A1402581603010007941 60A027E182E07BA180A02FE1A073A1B0A02
EC1D0E07281E0A02842107C0210A02062C2D07422C0A02483507843 50A0A0D03640008
00633E0A1402E015090D660C1702D4172E6600190290 1A66BC1B02B01D0E66781E0234
21090E66FC21025C2B2D090D66EC2C02BC3466E8350A0D03640008006710341D246400
1D1664001D12640000$$$$$
```

1.4. SAMPLE MEASUREMENT

This paragraph describes the various types of measurement possible when parameter lists, etc. have been assembled as described in paragraph 1.3.

Note that the basic microprocessor-controlled version produces a measurement readout of element gross intensities, but corrected by the electronic circuits for various effects such as dead-time, distortion of the detector pulses, position of the goniometer, etc. If concentration values are required the intensity data must be input to a calculator or computer, or the spectrometer must be connected to a PW 1790/10, P851 Computer (XR14 software developed for the PW1400 system is described in paragraph 2).

Measurements using the PW1500 sample loader or sample changer are described in paragraph 3.1. and 3.2.

1.4.1. General

Before list assembly can commence the PWR command must have been given. This command defines the maximum power (tube rating) and maximum kV (generator rating) that can be set by the kV and mA input during channel assembly. The command is not stored in the parameter bank and thus remains active provided that mains generated or battery power is supplied to the RAM card.

Before a start measurment command is given, the following commands can be given:

MSK	- selection of collimator mask (not needed before SMX)
SPN	- spinner on or off
CMD or BMD	- continuous or batch mode - see paragraph 1.4.5.
RCM, RCJ, MPY or RES	- repeat measurement commands and reset - see paragraph 1.4.6.
NRL, SOT, RMS, COM	- output device commands, as required.
SLP, ULM	- if required to unload samples from the turret. SLP is not required if SMX is used with sample identification
LDM	- given before SMM command to load a monitor sample.

ASC, and other sample loader and sample changer commands, refer to paragraphs 3.1 and 3.2.
Manual parameter settings must also be given, if required.

Start measurement commands

The following commands can be given to initiate the measurement procedure:

SMX i (j) (k)	Start measurement of unknown samples using MP lists i (j and k if input)
SMX	Start measurement using MP list(s) previously input.
i (j)(k)	Start measurement in SMX mode.

Note: More than three MP lists (i, j, k) can be input but only the first three will be measured.

c.r.	Start measurement in SMX mode using MP list(s) previously input.
SMM i (j)(k)	Start measurement of the monitor sample using the MP lists i (j and k if input). The MP list preset time and/or count will be multiplied by the factor input for MOMPY, see also ratio measurement paragraphs 1.4.3. and 1.4.4.

Measurement of unknown samples (SMX) will not commence until the sample loading positions, and identification if required, have been input - see the examples shown in paragraph 1.4.2. etc.

Sample identification

If a capital letter I is typed (SMX command) after the turret positions input, unknown samples can be given an identification, comprising up to 12 alpha-numeric characters, and this identification will be printed above the columns of element intensities in the readout.

If an I is not typed the microprocessor assumes that samples are already loaded in the turret, and the cap will not open. In this case, if samples are to be loaded, use the SLP command before SMX.

Samples loaded from a sample changer are not identified, but the sample tray and sample position numbers are printed in the results readout to allow manual identification of each sample if required.

1.4.2. Absolute measurement

The measurement of element intensities of samples in the absolute mode, should follow the procedure below:

- Assemble the required channel sets, and MP list (s).
  Note that ABS: = YE in the MP list assembly, see paragraph 1.3.2.
- Input any pre-measurement commands, such as CMD or BMD, or recycle.
- Type the start measurement command, see above.
- Load the sample(s), and type identifications as required. When the last c.r. is given the measurement(s) commences.
- After measurement, unload the samples and repeat the procedure as required.

Figure 1.4A shows a print of measurement program 10, which is used to measure an unknown sample. The result readout shows a listing of the counts and time for each channel (element line).

An example of a qualitative measurement is shown in paragraph 1.4.9.

```
C=PMP 10          Print measurement program 10

MP 10

MASK :  2
ABS  : YE

CHAN    PT    PC
FE      10   0E0
CA2     20   0E0
K        4   0E0
S       10   0E0
S+      10   0E0
SI      20   0E0
AL      20   0E0
MG2-    20   0E0
MG2     40   0E0
NA      40   0E0
NA+     20   0E0
C=
```

```
C=SMX 10
SAM.POS :=1 I
<1> :=C 2476/16
```

Start measuring unknown sample using MP10. Sample loaded in turret position 1, and identification required. Identification of sample, then measurement commences.

```
MP 10   1 SAMPLES 11 CHANNELS   MOPS   0
     1 : C 2476/16
FE      223907   10.000
CA2    5086238   20.000
K       387150    4.000
S       162937   10.000
S+        9951   10.000
SI      951626   20.000
AL      226884   20.000
MG2-      2099   20.000
MG2      22287   40.000
NA       21367   40.000
NA+       5360   20.000
C=
```

Figure 1.4A Absolute measurement of a sample.

1.4.3. Buffer ratio measurement

Ratio measurement uses specially prepared and chemically stable monitor sample(s), having a similar composition to the unknown samples to be measured. By measuring the monitor, and then the unknown samples, and calculating the ratio intensity for the unknown samples (see below), the effect of any drift of measurement results is reduced. It is normal to measure the monitor sample for a longer period to improve the counting statistics, and the monitor multiply factor (MOMPY) input is used for this purpose. Ratio measurements use either the "buffer ratio method" or the "direct ratio method" (see paragraph 1.4.4.).

The monitor sample is usually stored in the turret, in positions 1 to 3 depending on the measurement mode- batch or continuous, or whether a sample changer is used.

The sample measurement output from the microprocessor shows element total counts accumulated, and direct output of ratio intensities is not possible. The output of counts and time, for the monitor and the unknown samples, makes it possible for a calculator or computer to be programmed to produce ratio intensities and/or concentrations; refer to paragraph 2.

Buffer ratio measurement is possible when the MP list shows:
ABS = NO
BRAT = YE (yes)
MOPS = monitor sample loaded in turret position 1, 2 or 3
MOMPY = multiplication factor for PT and PC, on monitor sample measurement only.

The monitor sample must be loaded into the turret and measured before the unknown samples are measured. Use the load monitor command (LDM) giving the same turret position number as given for MOPS (see above). Then measure the monitor sample using the SMM command, and the same MP number(s) that will be used with the SMX command. Typical measurement results are shown in figure 1.4B, with a print of the MP list.

```
C=PMP 50          Print MP list 50

MP 50

MASK  :  1
ABS   : NO        Not absolute mode
BRAT  : YE        Buffer ratio chosen
MOPS  :  1        Monitor sample to use turret position 1
MOMPY :  2        Multiply PT and PC by 2 for monitor measurement

CHAN     PT    PC
MO       10   0E0  \
NB       10   0E0   )
NI       20   0E0   |
MN       10   0E0   | Channel measurement parameters
CR       20   0E0   |
TI        4   0E0   |
P2       10   0E0   )
S2       10   0E0  /
SI       20   0E0
C=
```

Print of measurement parameters list (figure 1.4B)

```
C=LDM 1          Load monitor sample in position 1
C=SMM 50         Measure the monitor sample using MP50

MP 50   0 SAMPLES   9 CHANNELS   MOPS   1
      1 : MONITOR
MO        77302   20.000
NB       104068   20.000
NI      1078669   40.000
MN        21098   20.000
CR      1247556   40.000
TI       152961    8.000
P2         1510   20.000
S2         1672   20.000
SI        89268   40.000
C=
```

Figure 1.4B Monitor measurement in the buffer ratio mode (including MP list)

It will be seen that the load monitor command does not start the measurement of the monitor sample. When the SMM command is given the monitor sample is automatically transferred to the measuring position, therefore be sure that the turret position defined by the LDM command is the same as the position given in the MP list assembly (MOPS =).

Note that in the example the measuring times are doubled because the monitor multiply factor MOMPY = 2 in the MP list.

The unknown samples can now be measured, and figure 1.4C shows that positions 2 and 3 are used, and each sample is identified. Turret position 1 is protected and cannot be used for the loading and measurement of unknown samples until an unload monitor command (ULM) is given.

The countrate ratio intensity R_i is given from:

$$R_i = \frac{ri\ (x)}{ri\ (m)}$$

, where ri (x) is the net element countrate (counts/measuring time), and ri (m) is the monitor countrate.

The results shown in figures 1.4B and 1.4C can be used to calculate the ratio intensity, using a calculator, or the result can be calculated automatically when a computer is connected, refer to paragraph 2.

```
C=SMX 50                 Start measurement of unknown samples, using MP50
SAM.POS :=2 3 1          Turret positions to be used, and identification to be given
<2> :=ST.STEEL #94       Sample identifcation
<3> :=ST.STEEL #35

MP 50   2 SAMPLES   9 CHANNELS   MOPS   0
      2 : ST.STEEL #94  3 : ST.STEEL #35
MO        19460   10.000     14603   10.000
NB        29864   10.000      8698   10.000
NI       375113   20.000    841468   20.000
MN        26908   10.000     28626   10.000
CR       233350   20.000    754886   20.000
TI        25435    4.000      7879    4.000
P2          651   10.000       879   10.000
S2          689   10.000       703   10.000
SI        24691   20.000     28263   20.000
C=


C=ULM 1          Unload monitor sample, position 1 can now be used to load uknown samples
```

Figure 1.4C Sample measurement in the buffer ratio mode

1.4.4. Direct ratio measurement

This method of ratio measurement varies from the buffer ratio method (see paragraph 1.4.3.) in that the monitor sample is not measured by a separate command (SMM not required), but is measured together with the unknown samples.

Direct ratio measurement is performed when the MP list assembly shows:
ABS = NO
BRAT = NO (or c.r. when BRAT . NO : = is printed)
MOPS = turret position number for monitor sample (1, 2 or 3)
MOMPY = multiplication factor for PT and PC, when the monitor sample is measured.

The microprocessor software controls the measurement in two ways:

1) To give an output which is a direct measure of the ratio intensity.
   This is possible when the **preset time (PT)** assembled in the MP list is **zero** (infinity), for the selected elements, i.e. for those elements to be measured in the direct ratio mode. The preset count value (between 1E4 and 5E7) must be given. In this case the **monitor multiplying factor (MOMPY) is not operative,** see figure 1.4D.
2) To give an output which requires separate calculation to determine ratio intensity, i.e. by using a caculator or a computer.
   For this mode the **preset time (PT) is not zero,** both PT and PC **must be used** and the **multiplying factor MOMPY is operative,** when the monitor sample is measured, see figure 1.4E.

In both cases the elements which are not required to be measured in the monitor sample have the preset count (PC) entered as zero in the MP list assembly. The preset time (PT) is used to stop the element measurement of the unknown sample, therefore, these elements are measured in the absolute mode.

The monitor sample must be loaded into the turret when the LDM command is given, and the turret position number must be the same as that given for the MOPS input during the MP list assembly. A separate monitor measurement command (SMM) is not input, and the monitor sample is measured first when the SMX command is given (after identification, etc.), but only for the elements with PT = 0.

Referring to figure 1.4D, the monitor sample measurement result shows the time required to accumulate the preset counts, but only for the element channels with PT = 0. The time for this measurement is used when the unknown sample is measured, so that the resulting count is now a measure of the ratio intensity. Since R_i = ri (x) / ri (m), then for zinc $R_i = 6842509/10^7 = 68.4\%$.

In the second case (figure 1.4E), the two elements in the monitor sample are measured for a preset time and preset count multiplied by MOMPY. Note that for zinc the preset count (2×10^7) occurs first, and for Cu2 the preset time (200 seconds) stops the measurement. The ratio intensity is calculated from the countrate determined from the monitor and unknown sample measurement, i.e. for zinc:
$R_i = (2.10^7/87.109)\ (10^7/63.659)^{-1} = 68{,}4\%$

```
C=LDM 1          Load monitor
C=SMX 41         Start measurement (monitor and unknown samples) after identification .
SAM.POS :=2 1
<2> :=BRASS SP.604

MP 41   1 SAMPLES   8 CHANNELS   MOPS   1
      1 : MONITOR         2 : BRASS SP.604
SN            0     .000     58123   10.000
PB            0     .000     22679   10.000
ZN     10000000   43.550   6842509   43.550 }  Unknown samples measured for a time
CU2    10000000  151.431  10418725  151.431 }  determined from the monitor
NI            0     .000     28884    4.000    measurement.
FE            0     .000     21746    4.000
MN            0     .000     30627   10.000
AL            0     .000      7550   10.000
C=

  /

C=PMP 41         Print MP list 41

MP 41

MASK :  1
ABS  : NO  }
BRAT : NO  }     Direct ratio mode selection
MOPS :  1
MOMPY:  1

CHAN    PT    PC
SN      10   0E0
PB      10   0E0
ZN       0   1E7 }  Direct ratio mode elements, remainder are to be measured in the absolute mode.
CU2      0   1E7 }
NI       4   0E0
FE       4   0E0
MN      10   0E0
AL      10   0E0
C=ULM 1          Unload monitor sample
C=
```

Figure 1.4D Direct ratio mode measurement of two elements, with readout indicating ratio intensity

```
C=LDM 1
C=SMX 42
SAM.POS :=2 1
<2>  :=BRASS SP.604

MP 42   1 SAMPLES   8 CHANNELS   MOPS   1
      1 : MONITOR          2 : BRASS SP.604
SN              0     .000      57921   10.000
PB              0     .000      2...9   1...900
ZN       20000000   87.109  10000000   43.659 } Ri = ri (x) /ri (m)
CU2      13207909  200.000   6880560  100.000 }
NI              0     .000      29123    4.000
FE              0     .000      21740    4.000
MN              0     .000      31031   10.000
AL              0     .000       7632   10.000
```

Monitor PT/PC multiplied by MOMPY

```
C=FMP 42

MP 42

MASK :   1
ABS  : NO  } Direct ratio mode selection
BRAT : NO  }
MOPS :   1
MOMPY:   2     Note monitor multiplying factor

CHAN    PT    PC
SN      10   0E0
PB      10   0E0
ZN     100   1E7  } Direct ratio mode elements
CU2    100   1E7  }
NI       4   0E0
FE       4   0E0
MN      10   0E0
AL      10   0E0
C=
```

Figure 1.4E Direct ratio mode measurement (requiring further calculation to determine ratio intensity)

1.4.5. Continuous/Batch measurement mode

The order in which samples are loaded and measured is determined by the mode command CMD or BMD. The selected command must be given before the start measurement command, and it remains active until the other mode is chosen. When a sample changer is installed, both commands can be superceded by the ASC command, refer to paragraphs 1.4.12., 3.1 and 3.2.

When the continuous measurement mode is chosen, samples are loaded and measured alternately in turret positions 2 and 4.

When the batch measurement mode is chosen, up to four samples are loaded and identified before the measurement commences.

Ratio measurements are possible in either mode, but an error message will be output if an attempt is made to load an unknown sample into a protected (monitor) turret position.

Continuous mode measurement.

In the continuous mode, when the SMX command is given, the sample turret will rotate until position 2 or 4 is at the loading position and the cap will open. The sample can be loaded and identified, and when the carriage return is given the turret rotates and brings the sample to the measuring position. Measurement commences and the result is printed.

During measurement the cap at the loading position opens (no turret rotation), and a further sample can be loaded after taking out the previously measured sample. Note that during continuous measurement /C can be given after a sample is loaded. This causes the cap to close and the sample will pass through the airlock onto the turret.

Another start measurement command is given. (SMX i, i, or c.r.), and the sample identification is given for the newly loaded sample. After c.r. the turret rotates 180^{o}, measurement commences, results are printed, and the cap opens. The first sample can be removed and replaced by another sample.

The cycle is repeated, start measurement command, identification, etc. until all samples are measured. The last sample can be removed using the SLP command.

An example of the continuous mode measurement is shown in figure 1.4F.

```
C=CMD                    Continuous measurement mode selected
C=SMX 10                 Start measurement with MP10
<4> :=C 2476/18          Turret position 4 to LP, cap up, load sample and identify

MP 10   1 SAMPLES 11 CHANNELS   MOPS   0
     4 : C 2476/18
FE       210764   10.000
CA2     5047597   20.000
K        353838    4.000
S        190862   10.000
S+        10251   10.000
SI       939307   20.000
AL       221227   20.000
MG2-       2068   20.000
MG2       21022   40.000
NA        20938   40.000
NA+        5210   20.000   During measurement cap opens (no turret rotation).
C=10                       Choose MP10, same mode
<2> :=C 2476/19            Load sample into position and identify

MP 10   1 SAMPLES 11 CHANNELS   MOPS   0
     2 : C 2476/19
FE       227096   10.000
CA2     5080882   20.000
K        308545    4.000
S        169725   10.000
S+         9973   10.000
SI       964112   20.000
AL       235965   20.000
MG2-       2008   20.000
MG2       21564   40.000
NA        23494   40.000
NA+        5356   20.000   Unload first sample, insert new sample,
C=                          c.r. chooses same mode and MP list
<4> :=C 2476/20            Sample identification, after c.r. turret rotates 180°

MP 10   1 SAMPLES 11 CHANNELS   MOPS   0
     4 : C 2476/20
FE       224390   10.000
CA2     5062622   20.000
K        386249    4.000
S        163067   10.000
S+        10029   10.000
SI       945025   20.000
AL       224931   20.000
MG2-       2116   20.000
MG2       21931   40.000
NA        21393   40.000
NA+        5351   20.000
C=
```

Figure 1.4F Continuous mode measurement

Batch mode measurement

When the SMX command is given in the batch mode, an input of turret positions (1 to 4) and optional identification (I) is required. If I is not input the software assumes that the samples are already loaded into the turret, and the cap will not open. Therefore, the operator will have to give the SLP command and load the sample, for each turret position to be filled. Then the SMX command can be given.
The same situation exists when the measurement is controlled by a job listing, and all mechanical actions, such as sample loading, must be carried out before the start job measurement command.

When I is given the turret position with the lowest number (as input for the SMX command) is brought to the loading position. For example, if:
SMX 10
SAM.POS: 3 1 4 2 I, is input, the turret loading positions order will be 1, 2, 3 and 4.
The cap opens for each sample loading, and after sample identification the cap comes down, the turret rotates to the next lowest position number, and the procedure repeats. After the final c.r. the measurement of the first sample commences, and is followed by the measurement of the remaining samples in the turret. After the final sample is measured the results are output element by element, see figure 1.4G.

The samples can be unloaded using the SLP command, or by using a further start measurement command when the previously measured samples can be replaced by fresh samples.

```
C=BMD                    Batch measurement mode selected
C=SMX 10                 Start measurement with MP10
SAM.POS :=1 2 3 4 I      Samples to be loaded in turret positions 1,2,3, and 4 and identified
<1> :=CEMENT
<2> :=CLINKER            Turret to loading position 1, cap up, insert sample and identify. After
<3> :=KILN SLURRY        c.r., cap down, turret rotates to LP2, cap up, and procedure repeated.
<4> :=LIMESTONE
```

```
MP 10   4 SAMPLES 11 CHANNELS   MOPS  0
      1 : CEMENT          2 : CLINKER          3 : KILN SLURRY   4 : LIMESTONE
FE      224446   10.000    222298   10.000     184563   10.000    114850   10.000
CA2    5085685   20.000   5210505   20.000    5007536   20.000   5814292   20.000
K       389092    4.000    382981    4.000     445104    4.000    217609    4.000
S       162965   10.000     21814   10.000      17993   10.000     12859   10.000
S+        9994   10.000      9639   10.000       8908   10.000     10023   10.000
SI      949725   20.000   1027231   20.000     614137   20.000    248233   20.000
AL      226322   20.000    225412   20.000     138052   20.000     57787   20.000
MG2-      2100   20.000      2080   20.000       1876   20.000      2140   20.000
MG2      22324   40.000     24920   40.000      15029   40.000     16816   40.000
NA       21275   40.000     19685   40.000      15720   40.000     12830   40.000
NA+       5386   20.000      5285   20.000       4874   20.000      5305   20.000
C=
```

Figure 1.4G Batch mode measurement

1.4.6. Recycle and time/count multiplication

It is possible to repeat a measurement by giving a recycle command, or to apply a multiplying factor to the MP list preset time and count values. The command will remain active until reset (RES command), and should be input before the start measurement (SMX) command.

Recycle measurements.

The repeated measurement of a sample will provide information on the precision of the measurement.

Command RCM i will recycle the measurement program i times, where i = 0 to 127. If i = 0 the recycle operation will continue until reset, or until a slash is given (when the command is still active). An example of the recycle command is shown in figure 1.4H.

```
C=RCM 3                 Recycle the following measurements three times
C=SMX 10                Start measurement of program 10
SAM.POS :=1 I
<1> :=C 2476/17

MP 10   1 SAMPLES 11 CHANNELS   MOPS   0   CYCLE    1
      1 : C 2476/17
FE       218493   10.000
CA2     5059256   20.000
K        310577    4.000
S        148413   10.000
S+         9884   10.000
SI       957228   20.000      First set of measurement results
AL       230024   20.000
MG2-       2123   20.000
MG2       20185   40.000
NA        22803   40.000
NA+        5318   20.000

MP 10   1 SAMPLES 11 CHANNELS   MOPS   0   CYCLE    2
      1 : C 2476/17
FE       218997   10.000
CA2     5058744   20.000
K        310095    4.000
S        148376   10.000
S+         9916   10.000      Second measurement of same sample with
SI       956886   20.000      existing measurement program
AL       229372   20.000
MG2-       2030   20.000
MG2       20448   40.000
NA        23015   40.000
NA+        5331   20.000

MP 10   1 SAMPLES 11 CHANNELS   MOPS   0   CYCLE    3
      1 : C 2476/17
FE       218763   10.000
CA2     5059748   20.000
K        309095    4.000
S        148200   10.000
S+         9915   10.000
SI       957056   20.000      Final measurement
AL       230619   20.000
MG2-       2084   20.000
MG2       20394   40.000
NA        22935   40.000
NA+        5169   20.000
C=                             Back to normal dialog
```

Fig. 1.4H. Recycle of sample measurement.

Count/time multiplied measurement.

If the length of a measurement is increased the counting statistical precision will improve. The existing measurement program list need not be changed to increase the measurement time, instead a multiplication factor command can be given.

Command MPY i will multiply the preset time (PT) and preset count (PC) values in the measuring programs selected by a subsequent start measurement (SMX) command. The factor i can be 1, 2, 4, 10, 20 or 40. The command remains active until reset (RES command), which will also reset RCM, RCJ, RCS and ASC.

A calculator or computer can be used to determine the average countrate from the counts and time readout for each element - see figure 1.4.J.

Note that the measurement program lists can be assembled with a monitor multiply factor, which multiplies PT and PC in the list for **monitor measurement only.**

Note also that the use of a multiply factor can cause overflow of the time and counts registers in the spectrometer, depending on the preset stop conditions (PT or PC). In the case of an overflow an indication is not given, but the counter is reset and continues from zero again. The capacity of the counters is sufficiently high that any overflow will be apparent and can be noted. Overflow takes place when the time counter reaches 1000 seconds, and the counts reaches 10^8. If a PT or PC value is not entered during the MP list assembly, a value of zero is taken, which means infinity.

```
C=MPY 2          Multiply factor = 2
C=SMX 10         Start measurement of program 10
SAM.POS :=1 I
<1> :=C 2476/21

MP 10  1 SAMPLES 11 CHANNELS  MOPS  0
     1 : C 2476/21
FE      453482  20.000
CA2   10162546  40.000
K       615961   8.000
S       341037  20.000
S+       20035  20.000
SI     1938916  40.000
AL      477321  40.000
MG2-      4302  40.000
MG2      43037  80.000
NA       47138  80.000
NA+      10748  40.000
C=PMP 10

MP 10

MASK :  2
ABS  : YE

CHAN    PT    PC
FE      10   0E0
CA2     20   0E0
K        4   0E0
S       10   0E0
S+      10   0E0
SI      20   0E0
AL      20   0E0
MG2-    20   0E0
MG2     40   0E0
NA      40   0E0
NA+     20   0E0
C=
```

Measuring times multiplied by a factor of two, refer to MP10 preset times below.

Fig. 1.4J. Measurement using the multiply factor.

1.4.7. Job measurement

The variety of jobs which can be assembled is too wide to be fully described, but an example of a job measurement using step scans, and one using continuous scans are shown in figures 1.4K and 1.4L.

Firstly, a job must be assembled as described in paragraph 1.3.3. Take care in assembling a job as it cannot be changed, only deleted and then re-assembled. If an error is made during the assembly, the typed character(s) or whole line can be deleted by using a long dash — or ^ , refer to paragraph 1.1.1. as long as c.r. is not yet given. Also note that a job list program must not exceed 255 bytes, or an error message will be printed (see paragraph 1.2.1.), and list assembly is inhibited.

Measurement using a job list is started from the command SJB i, where i = 1 to 63. The start of a job measurement from a tray identifciation card in the sample changer is described in paragraph 3.1./3.2. Repeated job measurement is described in paragraph 1.4.8.

Figure 1.4K shows a typical readout of the measurement of a sample, where the goniometer step scans between the angles defined in a job list (number 34). This job list also defines various other conditions, such as preset time setting (PTS), filter in (FLT Y), collimator coarse (COL C), slew fast (SLF —), etc.

Figure 1.4L shows a similar readout, but this time the sample is measured with continuous scans, and peak shapes are defined by plotting the output on a chart recorder (with a change of full-scale range)

1.4.8. Recycle job measurement.

A complete cycle of job measurement can be repeated using the command:

RCJ i	Recycle the job measurement i times, where i = 0 to 127, and 0 means infinite. When 0 is given the cycle number printed in the output goes to 255 maximum; then prints from 0 again.

The RCM and/or MPY commands (paragraph 1.4.6) can be included with the RCJ command, for example, each job cycle can include repeated sample measurements.

The RCJ command remains active until reset by:

RES	Reset recycling command RCJ (also RCM, MPY, RCS and ASC).

Recycle can also be reset by typing RCJ 1.

```
C=SJB 34
```

Start job 34

Assemble job 34

```
C=AJB 34
```

```
JB 34
 57.520         0     .000  FE
 57.200         0     .000
 57.200       578     .100
 57.300      1778     .100
 57.400      4431     .100
 57.500      5914     .100
 57.600      4754     .100
 57.700      2486     .100
 57.800       965     .100
 62.700         0     .000
 62.700      1270     .100
 62.800      3888     .100
 62.900      7556     .100
 63.000      8429     .100
 63.100      5933     .100
 63.200      2907     .100
 63.300      1119     .100
 69.100         0     .000
 69.100       197     .100
 69.200       510     .100
 69.300       805     .100
 69.400       877     .100
 69.500       568     .100
 69.600       271     .100
 69.700       110     .100
 76.600         0     .000
 76.600       376     .100
 76.700       939     .100
 76.800      2095     .100
 76.900      3239     .100
 77.000      3434     .100
 77.100      2961     .100
 77.200      2819     .100
 85.800         0     .000
 85.800      1220     .100
 85.900      3549     .100
 86.000      8172     .100
 86.100     12498     .100
 86.200     12980     .100
 86.300      9772     .100
 86.400      5865     .100
112.700         0     .000
112.700      2238     .100
112.800      5329     .100
112.900      6887     .100
113.000      8279     .100
113.100      9113     .100
113.200      8480     .100
113.300      7087     .100
136.400         0     .000
136.400      4404     .100
136.500      5284     .100
136.600      5956     .100
136.700      6073     .100
136.800      5866     .100
136.900      5258     .100
137.000      4270     .100
136.690         0     .000  K
136.690    608507   10.000
C=
```

Step scan over FeKα peak

MnKα

CrKα

VKα

TiKα

CaKα

KKα

Integrated counts in potassium channel

```
J=SCH FE
J=SLF 57.2
J=PTS .1
J=STS 57.8 .1
J=SLF 62.7
J=FLT Y
J=STS 63.3 .1
J=SLF 69.1
J=STS 69.7 .1
J=SLF 76.6
J=FLT N
J=STS 77.2 .1
J=SLF 85.8
J=STS 86.4 .1
J=SLF 112.7
J=COL C
J=STS 113.3 .1
J=SLF 136.4
J=STS 137.0 .1
J=SCH K
J=PTS 10
J=SCT
J=EJB

C=
```

Figure 1.4K Job assembly and measurement readout (with step scans)

1.4.7. Job measurement

The variety of jobs which can be assembled is too wide to be fully described, but an example of a job measurement using step scans, and one using continuous scans are shown in figures 1.4K and 1.4L.

Firstly, a job must be assembled as described in paragraph 1.3.3. Take care in assembling a job as it cannot be changed, only deleted and then re-assembled. If an error is made during the assembly, the typed character(s) or whole line can be deleted by using a long dash — or ^, refer to paragraph 1.1.1. as long as c.r. is not yet given. Also note that a job list program must not exceed 255 bytes, or an error message will be printed (see paragraph 1.2.1.), and list assembly is inhibited.

Measurement using a job list is started from the command SJB i, where i = 1 to 63. The start of a job measurement from a tray identifciation card in the sample changer is described in paragraph 3.1./3.2. Repeated job measurement is described in paragraph 1.4.8.

Figure 1.4K shows a typical readout of the measurement of a sample, where the goniometer step scans between the angles defined in a job list (number 34). This job list also defines various other conditions, such as preset time setting (PTS), filter in (FLT Y), collimator coarse (COL C), slew fast (SLF —), etc.

Figure 1.4L shows a similar readout, but this time the sample is measured with continuous scans, and peak shapes are defined by plotting the output on a chart recorder (with a change of full-scale range)

1.4.8. Recycle job measurement.

A complete cycle of job measurement can be repeated using the command:

RCJ i	Recycle the job measurement i times, where i = 0 to 127, and 0 means infinite. When 0 is given the cycle number printed in the output goes to 255 maximum; then prints from 0 again.

The RCM and/or MPY commands (paragraph 1.4.6) can be included with the RCJ command, for example, each job cycle can include repeated sample measurements.

The RCJ command remains active until reset by:

RES	Reset recycling command RCJ (also RCM, MPY, RCS and ASC).

Recycle can also be reset by typing RCJ 1.

```
C=SJB 34
```

Start job 34

Assemble job 34

```
C=AJB 34
```

```
JB 34
 57.520         0     .000  FE
 57.200         0     .000
 57.200       578     .100
 57.300      1778     .100
 57.400      4431     .100
 57.500      5914     .100
 57.600      4754     .100
 57.700      2486     .100
 57.800       965     .100
 62.700         0     .000
 62.700      1270     .100
 62.800      3888     .100
 62.900      7556     .100
 63.000      8429     .100
 63.100      5933     .100
 63.200      2907     .100
 63.300      1119     .100
 69.100         0     .000
 69.100       197     .100
 69.200       510     .100
 69.300       805     .100
 69.400       877     .100
 69.500       568     .100
 69.600       271     .100
 69.700       110     .100
 76.600         0     .000
 76.600       376     .100
 76.700       939     .100
 76.800      2095     .100
 76.900      3239     .100
 77.000      3434     .100
 77.100      2961     .100
 77.200      2819     .100
 85.800         0     .000
 85.800      1220     .100
 85.900      3549     .100
 86.000      8172     .100
 86.100     12498     .100
 86.200     12980     .100
 86.300      9772     .100
 86.400      5865     .100
112.700         0     .000
112.700      2238     .100
112.800      5329     .100
112.900      6887     .100
113.000      8279     .100
113.100      9113     .100
113.200      8480     .100
113.300      7087     .100
136.400         0     .000
136.400      4404     .100
136.500      5284     .100
136.600      5956     .100
136.700      6073     .100
136.800      5866     .100
136.900      5258     .100
137.000      4270     .100
136.690         0     .000  K
136.690    608507   10.000
C=
```

Step scan over FeKα peak

MnKα

CrKα

VKα

TiKα

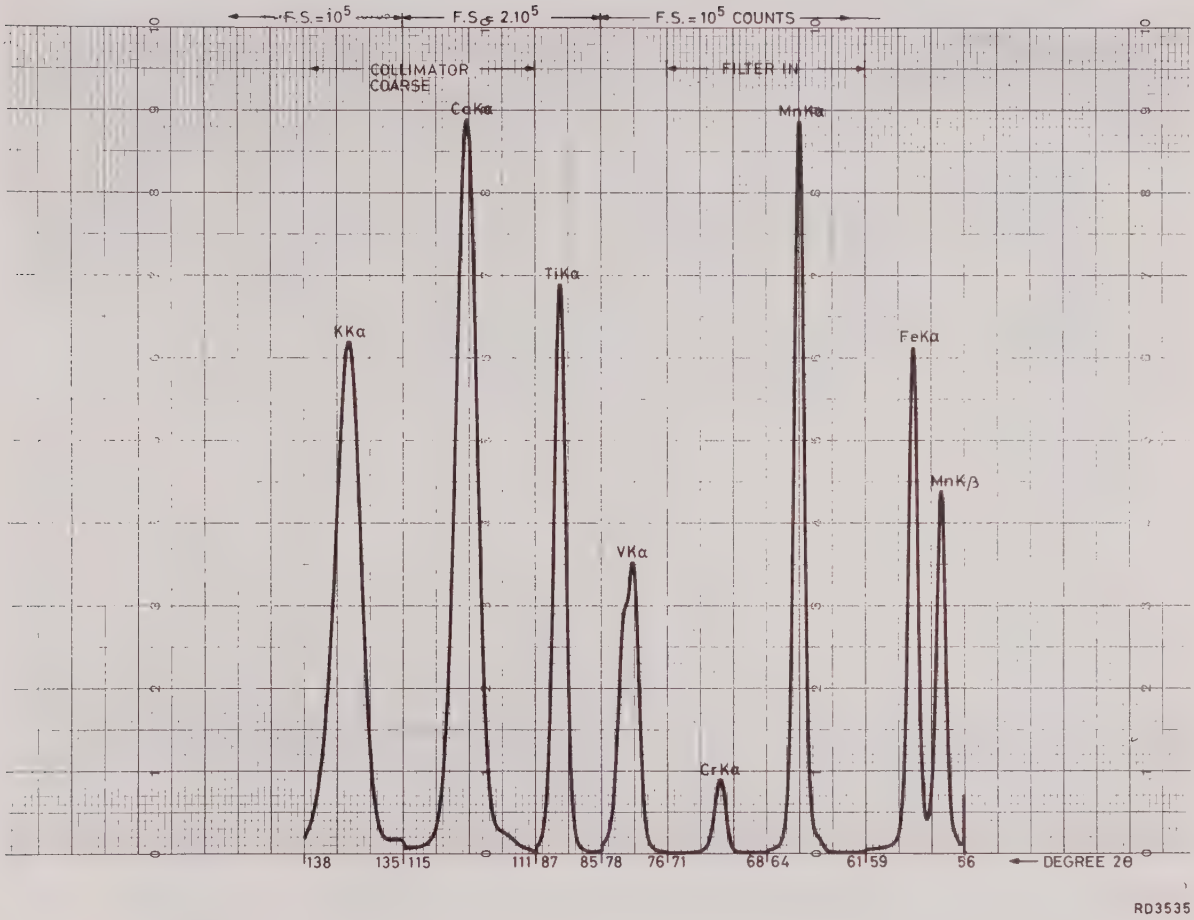
CaKα

KKα

Integrated counts in potassium channel

```
J=SCH FE
J=SLF 57.2
J=PTS .1
J=STS 57.8 .1
J=SLF 62.7
J=FLT Y
J=STS 63.3 .1
J=SLF 69.1
J=STS 69.7 .1
J=SLF 76.6
J=FLT N
J=STS 77.2 .1
J=SLF 85.8
J=STS 86.4 .1
J=SLF 112.7
J=CDL C
J=STS 113.3 .1
J=SLF 136.4
J=STS 137.0 .1
J=SCH K
J=PTS 10
J=SCT
J=EJB

C=
```

Figure 1.4K Job assembly and measurement readout (with step scans)



C=SJB 35 Start job measurement list 35

```
JB 35
 57.520          0      .000   FE
 56.000          0      .000 }
 59.000    1146369    89.932 }
 61.000          0      .000 }
 64.000    1010329    89.930 }
 68.000          0      .000 }
 71.000     112539    89.932 }
 76.000          0      .000 }
 78.000     669341    59.932 }
 85.000          0      .000 }
 87.000    1801230    59.932 }
111.000          0      .000 }
115.000    2179865   119.931 }
135.000          0      .000 }
138.000    1826902    89.932 }
136.690          0      .000   K
136.690     607256    10.000
C=
```

Iron channel setting

Continuous scan over Fe Kα

MnKα

CrKα

VKα

TiKα

CaKα

KKα

K channel counts for 10 seconds

Fig. 1.4L. Job printer and recorder readout (with continuous scans).

1.4.9. Manually controlled measurement

Sample measurements can be made from the input of single commands to define particular parameters. The counter/timer commands are used to preset time and/or counts, and to control measurement at fixed or variable goniometer positions. Figure 1.4M shows a typical example of a manually controlled measurement, involving turret operation (paragraph 1.6.4), goniometer and counter/timer operation, and change of parameters (paragraph 1.6.1.).

```
C=SLP 3          Turret position 3 to load sample
C=SMP 3          Sample in position 3 to measuring position
C=SLF 45         Slew fast (goniometer) to 45°2θ
C=PTS 1          Preset time to 1 second
C=SCT            Start counter/timer
 45.000   275490   1.000   Measurement result
C=COL C                   Now use coarse collimator
C=SCT                     Start measurement
 45.000   710232   1.000   Note increased counts
C=COL F                   Collimator fine
C=DET FS                  Use flow and scintillation detector
C=SCT                     Start measurement
 45.000   369497   1.000   Counts using both detectors
C=DET F                   Flow detector only
C=SLF 46                  Goniometer angle = 46°2θ
C=SCT                     Start measurement
 46.000      900   1.000   Low intensity result
C=PTS 20                  Preset time now 20 seconds
C=SCT                     Start measurement
 46.000    18105  20.000   20 times higher counts — improved statistics
C=SLF 47.345              Set goniometer to background angle
C=SCT                     Start measurement
 47.345     7239  20.000   Background intensity
C=
```

Figure 1.4M Typical measurement under manual control.

Counter/Timer

The following commands are given to preset the count/time measurement conditions, and to start the counter/timer circuit. They will normally be used in conjunction with other commands, such as SCH, STS, etc.

PTS t — Preset time to t seconds, where t = 0 to 999.9 in 0.1 steps.
A preset time setting will cause the preset counts to go to maximum (if PCS is not input), and vice-versa.

PCS iEj — Preset count to iEj, where
i = 1, 2, 5 or 0 (0 = infinity)
E = exponential
j = 4 to 7
Thus, the count range is 10 000 to 50 000 000, or infinity.

PTC t iEj — Preset time and counts, where the t and iEj values are as shown for PTS and PCS. Counting will stop when the first condition is reached, see figure 1.4.N.

SCT — Start counter/timer - measurement will commence.

Goniometer scanning

Step or continuous scanning through defined two-theta angles is controlled from the following commands. Note that goniometer position commands SLF, SLS and SSM are described in paragraph 1.6.2.

STS x ss — Step scan from the current goniometer angle to angle x^{o}, with a step size of ss^{o} 2θ. The period per step is defined by the previously input counter/timer command.
x = 0 to 147^{o} 2θ in 0.005 steps, and
ss = .005 to $.635^{o}$ 2θ in 0.005 steps.

Two step scan examples are shown in figure 1.4N, with different stop conditions for the steps, also see figure 1.4K.

CTS x s — Continuous scan from the current goniometer angle to the defined angle x^{o}, with a scanning speed of s degrees per minute.
x = 0 to 147^{o} (as for STS)
s = 0.25, 0.5, 1, 2, 4, 8, 16 or 32 degrees two-theta per minute.

Figure 1.4P shows a continuous scan from 40 to 47^{o} with a printer output and a chart recorder output. The printer output shows the final angle (x^{o}), the accumulated counts, and the total time of the measurement. Note that the product of time constant setting and chart paper speed should be ≈ 1.

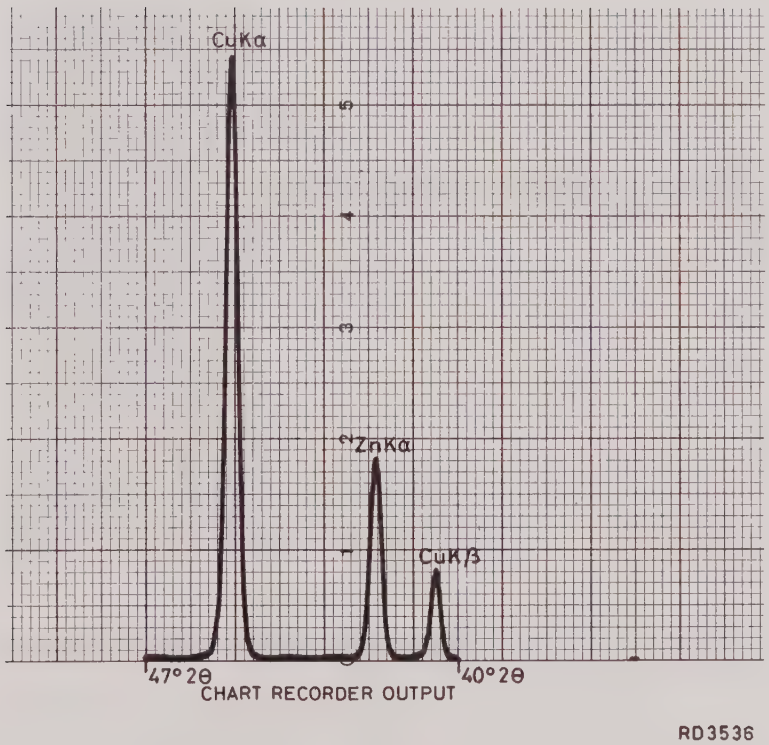
```
C=PTS 1                    Preset time setting (1second)
C=SLF 44                   Slew fast to 44°2θ
C=STS 46 .1                Step scan to 46° with 0,1°/step
 44.000        436    1.000
 44.100        491    1.000
 44.200        576    1.000
 44.300        845    1.000
 44.400       1444    1.000
 44.500       2921    1.000
 44.600       6987    1.000
 44.700      19065    1.000
 44.800      57795    1.000
 44.900     142932    1.000
 45.000     211366    1.000
 45.100     198159    1.000
 45.200     130696    1.000
 45.300      69234    1.000
 45.400      31686    1.000
 45.500      12690    1.000
 45.600       4915    1.000
 45.700       2168    1.000
 45.800       1321    1.000
 45.900        941    1.000
 46.000        751    1.000
C=/
```

```
C=PTC 1 1E5                Preset time and count (1 second and 10^5 counts)
C=SLF 44                   Slew fast to 44°2θ
C=STS 46 .1                Step scan to 46°2θ with 0,1°/step
 44.000        391    1.000      Preset time occurs first
 44.100        500    1.000
 44.200        632    1.000
 44.300        870    1.000
 44.400       1448    1.000
 44.500       3020    1.000
 44.600       6911    1.000
 44.700      19212    1.000
 44.800      57747    1.000
 44.900     100000     .699 }
 45.000     100000     .471 }  Stop condition from the preset count input
 45.100     100001     .503 }  (PTC command)
 45.200     100000     .763 }
 45.300      69059    1.000
 45.400      31617    1.000
 45.500      12730    1.000
 45.600       4824    1.000
 45.700       2139    1.000
 45.800       1285    1.000
 45.900       1011    1.000
 46.000        809    1.000
C=
```

Figure 1.4N Step scan with preset time, and with preset time/count.

Full scale = 5.10^4 counts

= 5E4




```
C=SLF  3        Sample turret position 3 to loading position
C=SMF  3        Sample turret position 3 to measuring position
C=RMS  5E4      Recorder full-scale to 50 000 counts
C=SLF  40       Slew fast to 40°2θ
C=CTS  47  2    Continuous scan to 47°, at 2°/minute
 47.000    395175  209.930    Final angle, counts and time
C=
```

Figure 1.4P Manually controlled continuous scan.

1.4.10 Angle calibration

The calibrate angle command (CAN) can be given to automatically check the peak goniometer setting of a channel. This routine should be followed for example if a crystal has been re-aligned, also see paragrahp 6.4.

Load a suitable sample, and bring it to the measuring position.
Select the appropriate mask (as selected in the MP list).

Give the CAN command, for the channel angle to be calibrated, and input the measurement time per step (in seconds), and the range of goniometer angle to be scanned.
TIME : 1.0 : = 0.1 to 999.9 in 0.1 steps (seconds)
RANGE : .20 : = 0.01 to 0.6 in 0.01 steps ($^{o}2\theta$).

The goniometer will go to the channel angle minus half the range input, and measure for the set time. The measurements are repeated at **0.005^{o} 2θ steps** up to the channel angle plus half the range angle. Every three sets of intensities are totalled in order to determine the peak goniometer angle, and this is printed in the output. The angle can be saved by giving a carriage return, and the ANGLE value of the channel set in the parameter bank is automatically updated. Type NO if the angle is not to be saved. If the calibrate angle routine is called for in a job measurement, a manual input is not allowed and the NEW ANGLE is automatically saved.

If the routine does not find a peak, the new angle is printed followed by three asterisk (!!!). If the range is one side of the element peak, the highest count angle will be printed, and the CAN routine should be repeated until a peak NEW ANGLE value is found. If the range is over a level characteristic and all intensities are the same value, e.g. a level background, the lowest angle value is printed.

```
C=PCH ZN        Print Zinc channel parameters (note goniometer angle)
ELEMENT FLT COL DET XTL ORD UPL LWL   KV  MA     ANGLE   +OFFS   -OFFS

ZN    KA  NO  F   F   1   1   75  25  60  50   41.800    1.00     .00


C=SLP 1
C=SMP 1
C=CAN ZN        Calibrate the goniometer angle of the zinc channel
TIME   : 1.0 :=4      Time of measurement of each 0.005° step is 4 seconds
RANGE  : .20 :=.05        Range of goniometer settings = 0.05° i.e. 41.775 to 41.825°2θ
ELMNT     MAX.SUM   OLD ANGLE   NEW ANGLE
  ZN      3344944      41.800      41.795      SAVE: YE :=New angle saved

C=PCH ZN  Print channel parameters to show new angle
ELEMENT FLT COL DET XTL ORD UPL LWL   KV  MA     ANGLE   +OFFS   -OFFS

ZN    KA  NO  F   F   1   1   75  25  60  50   41.795    1.00     .00
C=
```

Figure 1.4Q. Channel angle calibration.

1.4.11 Pulse height distribution

A record of the distribution of pulse heights for any element channel assembled in the parameter bank, can be printed as a listing of counts as the lower level varies from 0 to 100% , with a defined window width and time per step. If the time input is zero a chart recorder can be used to plot the distribution of intensities in the defined window as the lower level is varied. Typical outputs are shown in figures 1.4R and 1.4S. The results can be used to decide the channel lower level (LWL) and upper level (UPL) values, to fix the intensity and position of escape peaks, to check the resolution of the detectors,etc.

Proceed as follows:

- Load a suitable sample (SLP), and bring it to the measuring position. (SMP).
- Give the PHD command for the required channel, and input the width of the window to be used (in %), and the time for each window measurement. If the channel name is not given as an argument the recording will use the existing parameter set on the spectrometer (manual settings). With the lower level set to zero, the counts for the set time in the set window are measured: The lower level then advances to the next window measurement, and so on up to 100%. The readout shows a listing of these values, preceded by a measurement with the channel parameters for 1 second, i.e. with the normal UPL and LWL settings. The position of any peaks can easily be determined to allow the lower level and upper level to be set to suitable values for the channel.

To record the PHD analog readout, the chart recorder full-scale range must be set by typing the RMS command, after roughly checking the amplitude of the peaks of interest.

The chart recorder controls should be set before use, i.e. set paper speed, switch to INT, and adjust the paper position as required (pen down). Set the spectrometer time constant control (time constant times paper speed $\approx$ 1) and operate the COUNT RATE push-button.

Give the PHD command, with TIME input = 0, and the chart pen will trace an analog output similar to figure 1.4S. The rate at which the lower level value is advanced is determined by the chart recorder speed selection.A printer output is not given.

It is advisable to check the channel pulse height distributions when a gas bottle has been changed, or the flow counter cleaned or replaced.

The resolution of a detector can be determined when a p.h.d. curve is plotted , from the formula:

$$\text{Resolution} = \frac{\text{Full width at half maximum (FWHM)}}{\text{Average pulse height}}$$

From figure 1.4 S the % resolution $= 0{,}8/_{4{,}9} \times 100$

$\approx$ 16 %

```
C=PHD FE
WINDOW : 5 :=2
TIME : 1.0 :=
COUNTRATE     66969 CPS WITH UPL: 75 LWL: 20
%LL    COUNTS /    1.0 SEC
  0      2658
  2   2725617
  4       394
  6        24
  8        23
 10        22
 12        34
 14        20
 16        15
 18        24
 20        60
 22       321
 24      1011
 26      1572
 28      1277
 30       570
 32       260
 34       143
 36       125
 38       224
 40       632
 42      2599
 44      7307
 46     13510
 48     16279
 50     13505
 52      8087
 54      3715
 56      1289
 58       373
 60        98
 62        38
 64        32
 66        49
 68        34
 70        38
 72        45
 74        30
 76        24
 78        33
 80        27
 82        29
 84        31
 86        42
 88        36
 90        53
 92        48
 94        49
 96        25
 98        19
C=
```

Pulse height distribution for the iron channel

Window width = 2 %

Measurement time = 1 second

Measurement with normal channel settings

Pulse height distributions, with 2 % window for 1 second measurement, as lower level varies from 0 to 100 %

Fig. 1.4R. Pulse height distribution readout

```
C=RMS 2E4      Set recorder full-scale to 20 000 counts
C=PHD FE       Pulse height distribution for iron
WINDOW : 5 :=2 Window width = 2 %
TIME : 1.0 :=0 Zero time, therefore, chart recorder readout
C=
```

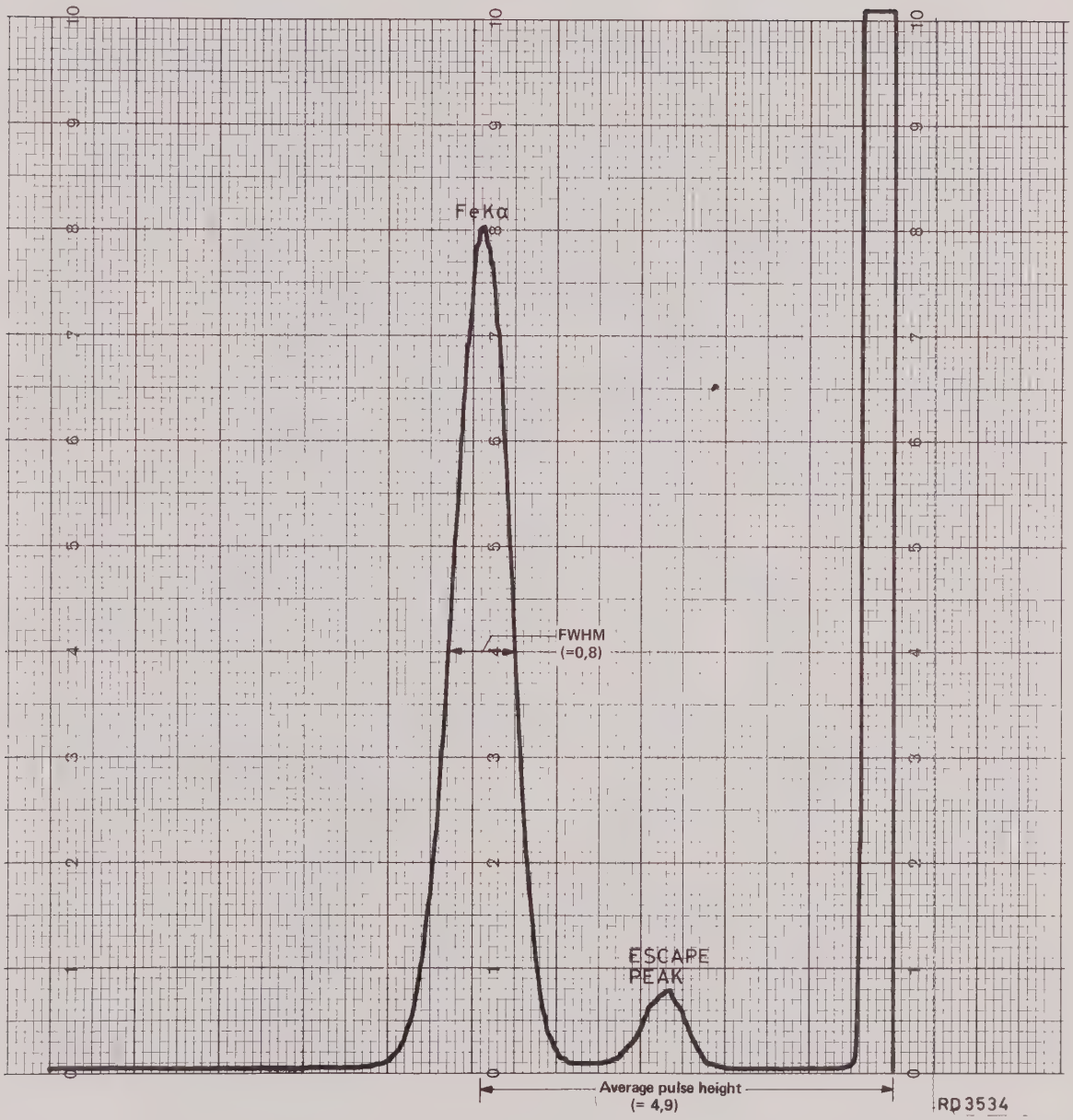


Fig. 1.4S. Chart recording of pulse height distributions.

1.4.12 Sample changer operation

When either the 6 position or 72 position sample changer is installed, the measurement of the samples can be controlled by operator typed commands, or by the coding of the identification card inserted in each sample tray.

Full details of the software commands, error messages, and the coding of the tray cards, are given in the Operation section of paragraphs 3.1. and 3.2.

Details of sampling handling in the spectrometer are given in paragraph 1.6.4.

1.5. RESULTS READ-OUT

When a measurement is finished the results will be output, and can be displayed or printed.
A variety of devices are available for connection to the PW 1400, and the operation is described in this paragraph. Details such as keyboard layout, jumper connections, etc. are described in paragraph 3.4., or see the Service Manual.

The main terminal is connected via an input/output interface circuit, and if a second interface circuit is installed a slave device (to receive output only) can be connected. One of the two terminals will probably be a printer to produce hard copy records.

If a computer is connected it will use the main input/output interface, and terminals connected to the computer will be used for all dialog, although a slave device can still be connected to the second interface.

The following commands can be given to control output to these devices:

NRL i — Number of lines per page, where i = 0, or 5 to 100 (0 means infinity). This command is intended for use with a V.D.U., see paragraph 1.5.2. and for most V.D.U. the number of lines is set to 24. The command remains active.

SOT a — Transmit data to a second output terminal, normally a printer, where a = Y (yes) or N (no output). The command remains active until cancelled by another SOT command.

COM — Communicate with the second output device. This command enables additional data to be transmitted to the second device (SOT must be given), as shown in figure 1.5A. Note that the COM command must be given for every line (80 characters maximum) of data.

- RMS iEj — Ratemeter (full-scale) setting to iEj, where
  i = 1, 2, 5 or 0 (automatic ranging)
  E = exponential
  j = 2 to 5
  i.e. range is 100 to 500 000 or automatic.

- This command can be used in a job list.

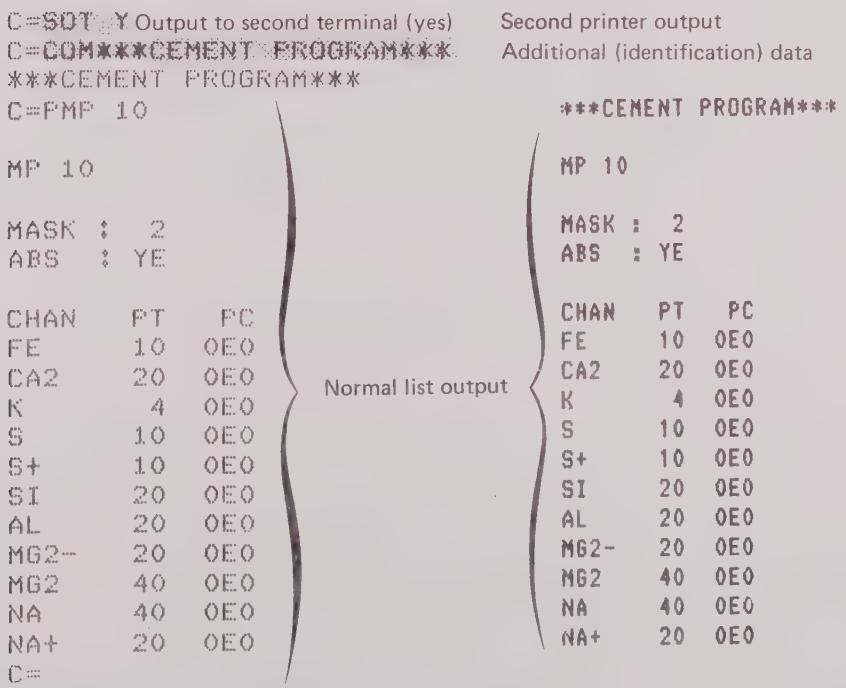


Fig. 1.5A. Output to a second printer, with additional (non-results) data

1.5.1. Printer

The PC 1409/00 Character printer is recommended for connection to the PW 1400. Operation of the keyboard is standard, and print-out is similar to the figures shown in this manual.

The typewriter key CAPS LOCK should be depressed, and the PARITY-OFF and DUPLEX-FULL push-buttons should be down — the remainder are normal (up). For normal PW 1400 operation the DATA lamp should be lit (if not,operate the push-button), but for off-line typing of information operate the LOCAL key (and the lamp will light — DATA extinguished).

If a V.D.U. is not connected, type NRL 0 to give continuous line printing.

1.5.2. Visual display unit

The P817-001 Video display terminal is used to display input and output data. Data appears at the bottom of the screen and moves upwards as new data is input, and it then spills over at the top of the screen and is lost. To avoid losing data when the PCH command is given, the command NRL i can be given previously. This defines the number of lines i per page, i.e. the maximum number of lines appearing on the screen.
When a page (screen) is full (lines = i) the message NEXT PAGE is displayed and further output is inhibited until a carriage return is given. Data display is resumed with new data at the bottom of the screen, until the screen is filled with the new data. Read-out can be terminated by a slash (/). For most VDU's the number of lines is 24.

An optional keyboard with numeric pad must be connected if the V.D.U. is the main terminal.

1.5.3. Chart recorder

A PM 8203/02 Chart recorder can be connected to record continuous scans made by the goniometer. The recorder will be in parallel with the front panel countrate meter, therefore, the COUNT RATE push-button must be operated (VACUUM out).

Before using the recorder set the full-scale range by the command RMS iEj, see above. The EXT/INT switch on the recorder must be set to INT, and external drive is not used. Operation of the remaining recorder controls is standard, and is described in the recorder manual.

The length and the resolution of the trace will depend on the goniometer scanning speed, the recorder chart speed, and the spectrometer ratemeter time constant. These parameters are interdependent and the optimum settings are determined by experience or trial and error. The following table will give general guidance:

Goniometer speed	Time constant	Paper speed cm/min.	
$^{o}2\theta$ /min.	seconds	*for 1^{o} 2θ = 1 cm*	*for 1^{o} 2θ = 2 cm*
1/8	$\leqslant$ 10	—	0.25
1/4	$\leqslant$ 4	0.25	0.5
1/2	$\leqslant$ 2	0.5	1
1	$\leqslant$ 1	1	2
2	0.5	2	4
4	0.5*	4	—

* only reliable for small peaks.

The time constant is set automatically if AUT is selected, and τ = 1000/counts range.
An event marker pen is deflected to indicate every $0{,}5^{o}2\theta$ goniometer angle movement.

1.5.4. Graphical terminal

A graphical terminal (such as the HP2648A with HP2613G graphical printer) can be connected, however, this type of terminal is primarily used when a computer is connected for PLOT readouts — see paragraph 2. It can be used for pulse height distributions and goniometer scans with the microprocessor only version.

1.5.5. Calculator connection

The connection and use of a calculator, for the processing of the intensity measurement results, will not be described in this manual.

1.6. SPECTROMETER OPERATION

This paragraph describes the application of the microprocessor software commands which are not used for routine analysis, i.e. commands not described in paragraphs 1.3, 1.4 and 1.5. The description of the purely hardware operation, e.g. vacuum system, is given in paragraph 5, but use of the associated panel controls is described in paragraph 1.6.5.

1.6.1. Parameter setting

The following commands can be used to set specific parameters for the manual measurement of a sample, or to check the operation of a parameter. For example, to examine the effect of changing a parameter, the procedure for sample measurement should follow the typical example shown in figure 1.6A. To check the operation of a parameter setting, input one of the following commands and check that the operation is correct on the display panel, for example, a change of crystal position, window setting, etc. is readily observed.

SCH xxi — Set the spectrometer conditions according to the channel set xxi previously input (command ACH). The display panel should indicate the spectrometer conditions, and the element intensity of a sample in the measuring position will be displayed on the countrate meter (COUNT RATE push-button operated).

SCH xxi ± — Parameters set as above, but with the goniometer offset (up or down) from the element 2θ angle (e.g. to a background position).

XTL i (i = 1 to 6)
ORD i (i = 1 or 2)
COL a (a = F or C)
FLT a (a = Y or N)
DET a (a = F, S or FS)
LWL i (i = 0 to 99)
UPL i (i = 0 to 99)
KVM ij (i = 25 to 100, j = 10 to 80)

} Value input can be checked on the display panel

All the above commands can be used in a job list assembly.

```
C=SCH FE      Set spectrometer to iron channel parameters
C=PTS 10      Preset time to 10 seconds
C=SCT         Start measurement
 57.520   116496   10.000   Note accumulated counts
C=COL C       Change collimator setting to coarse (C)
C=SCT         Start measurement
 57.520   321171   10.000   Note increased counts due to the selection of the coarse collimator
C=
```

Fig. 1.6A. Typical measurement with manually set parameters.

1.6.2. Goniometer positions

The following commands can be used to position the goniometer at required 2θ angles. The angle will be displayed on the front panel when the ANGLE push-button is operated.

- SLF x — Slew with a fast speed to goniometer angle x, where x = 0 to 147° 2θ in 0.005° steps. This operation uses the angle approach loop (see below).
- SLS x — Slew with a slow speed to angle x (x as for SLF). The goniometer drives directly to the angle and does not use the angle approach loop.

Commands SLF and SLS can be used in a job list assembly.

SSM ss — The goniometer makes a single step of ss degrees 2θ, where ss is .005 to .635° in multiples of .005°. A step is made every time a carriage return is given, and the initial direction is upwards (+), i.e. increasing angle.

The direction of movement can be reversed by typing – (or + if downward), and the step size can also be changed. The direction and step size remain active until a modification is input. A typical single step mode operation is shown in figure 1.6B, to set the goniometer at a peak angle. Note that the angle calibration (CAN command) is described in paragraph 1.4.10.

The angle approach loop circuit drives the goniometer at high speed (900°2θ per minute) to the required angle, and then deliberately overshoots. Slow speed drive (≈ 150°2θ per minute) is selected, and the final approach to the selected angle is always in an upward direction for a defined number of stepping motor pulses.

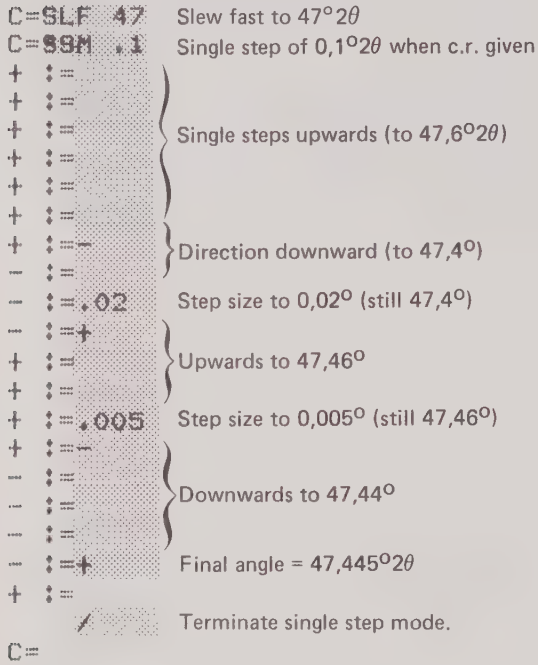


Figure 1.6B. Single step mode to set the goniometer to a peak angle.

1.6.3. Instrument conditions

The following commands set instrument conditions which are not normally changed.

PWR i k — Defines the maximum permitted programmed settings of generator power (i) and kilovolts (k), where i is 0 to 3 (kW), and k is 60 or 100 (kV). The command must be given when the PW1400 system is first used, and the values are stored in a RAM outside the parameter bank area, therefore, they will not be affected by the CPB command.

SPN a — Sets the sample spinner on (a = Y) or off (a = N). The spinner rotates at 30 rpm. Whenever the PW1400 is switched on, or reset, the spinner is switched on, but only runs when a sample is in the measuring position.

■ MSK i — Set the mask to position i, where i = 1 or 2. The command remains active until changed by a further command, or by the execution of an MP list by SMX or SMM command. The mask position, as specified in the MP list, will remain when the execution is completed. The size of the collimator mask can be 24 mm, 28 mm or 35 mm diameter, or 30 x 20 mm aperture, and the size fitted in positions 1 and 2 must be stated at installation.
This command can be used in a job list assembly.

1.6.4. Sample handling

The commands associated with the operation of the sample turret are described below, except for those which are used when a 6 position or 72 position sample changer is installed — see paragraphs 3.1 and 3.2.

SLP i — Rotate the designated turret position i to the loading position, where i = 1 to 4. The cap will open to allow a sample to be loaded in position i, and remains open until a start measurement or a SMP command is given.

▲ SMP i — Rotate turret position i to the measuring position. The cap closes and the turret rotates until the sample is under the X-ray tube.

▲ LDM i — Load a monitor sample in turret position i, where i = 1 to 3. The turret rotates, until position i is at the loading position, and a monitor sample can be inserted. This position is then protected against loading unknown samples. A warning will be given if a monitor measurement program is selected for ratio measurement (ABS = NO), but the LDM command has not been input.

▲ ULM i — Unload the monitor sample from turret position i. The LDM command is cancelled, and the turret position is no longer protected.

SMP, LDM and ULM can be used in a job list not selected by the changer identification card.

1.6.5. Panel controls

A few controls are situated on the spectrometer front panel and on the right-hand side panel (remove the side cover). The function of the lamps etc. of the synoptic display is self-explanatory, but detailed description is given in paragraph 5.

Chamber medium

At the left-hand side of the front panel the three push-buttons VACUUM/HELIUM/AIR will select the atmosphere to be present in the spectrometer chamber.
To change the atmosphere the existing depressed push-button must be pushed to release it, and the new selection can be made. Thus, it is not possible to select two push-buttons simultaneously. In the event that all push-buttons are normal (out), an error message "ERROR MEDIUM" will be generated when a sample measurement is attempted.

To select a **vacuum** medium (from an air or helium atmosphere), first remove the samples from the turret, particularly powder or liquid samples. Operate the VACUUM push-button (after releasing any other selection).

If a command (such as SMX) is given before the vacuum reaches ≈ 30 Pa, or if a vacuum leak is detected, an error message "ERROR VACUUM" is generated. The vacuum/countrate meter will show the amount of vacuum in pascals when push-button VACUUM is operated. The normal vacuum reading is less than 20 Pa (1 atm. ≈ 10^5 Pa).

To select a **helium** atmosphere in the spectrometer, first remove the air by selecting VACUUM. When the air is exhausted operate the HELIUM push-button. If necessary, to remove any trapped particles of air, the operation can be repeated, i.e. select VACUUM, and when evacuation is complete, select HELIUM. The helium gas flowrate is adjusted on the rear flow meter (on the side panel) to a flow of approximately 60 litres per hour.

The selection of an air atmosphere does not require any special procedure.

Measurement display

When the measurement of a sample commences the front panel will display the measurement program (MP) in use, and the element line being measured. Background and offset angle channels are not displayed in full, i.e. channel digits and + or — are not shown.

The upper right display will indicate counts, measuring time or goniometer angle when the relevant push-button is operated.

The meter and range display on the right-hand side will display vacuum or countrate when the relevant push-button is operated. The amount of vacuum is shown in pascals, and the digital display shows "UAC", which is the nearest possible indication for VAC. If COUNT RATE is selected the meter indicates the countrate (0 to 1) with the digital display multiplication factor. A green light AUTORANGING is lit when autoranging is operative e.g. when RMS 0 is used. When the count is less than 9%, or more than 101%, of the range in use, the range

Detector controls

The two potentiometers on the side panel will adjust the H.T. to the flow and scintillation detectors, refer to paragraph 6.1.

In addition the front flow meter will show the gas flow through the gas-flow detector. This is normally adjusted between 1 and 2 litres per hour.

The gas flow through the detector is monitored and if a fault condition is found (gas leakage) a message "ERROR DETECTOR GAS" is printed and operation is inhibited. This will also apply if the gas cylinder becomes empty. When the condition is rectified, the GAS LEAKAGE RESET push-button on the side panel must be operated to revert to normal operation.

Temperature stabilisation

The temperature control on the side panel sets the centre point of the proportional control circuit. The control covers a range of approximately 25 to 35 ^{o}C. The control should be set to the yearly average ambient temperature of the room and further adjustment should be avoided as accurate measurement and calibrations will be affected if the crystal "d" spacing changes.
If the cooling water is relatively warm, say 18-20 ^{o}C, the temperature control setting can be increased by a few degrees to avoid a high consumption of water in the cooling system.

H.T. Generator

The generator control settings, and the operation of the generator, are described fully in the Operation and Service Manuals supplied, but previous paragraphs in this manual detail the relevant operation.

(....)	means non-obligatory part of the command
i j k l m	mean integers
r	means a floating-point value
aaaa	means an element-name
XXXXXX	means a file-name
YYY	means the extension of the file
DEV:	means an output device (SY0:,SY1:,DX0:,DX1:)
yy	means number of iterations
tt	means tolerance

STOP POSSIBILITIES DURING A MEASUREMENT:

/ Emergency stop. Abort the measurement immediately and go to the command input mode.

/S Stop the scaler/timer, print the results and start the next run of the scaler/timer (if there is a next measurement programmed).

/M Stop after the complete measurement of the samples loaded in the sample turret. Used to interrupt a recycling program or to interrupt a measurement with the automatic sample changer.

/T Stop after the complete measurement of the present sample tray. To be used only if the sample changer is in operation. This command is only possible with Philips sample changer.

ACD (i)	Assemble Concentration-Data. If i is not given, the program starts with sample 1. If i is given, the program starts from sample i on.
ACH (xxi)	* Assemble CHannel xxi. The first x must be a letter and the second x must be a letter or may be absent , i is 1-3 or a space. The name DL must not be used, because it is used to delete a channel in a MP list and in a number of computer lists. There are a maximum of 63 channelsets. Example: ACH CU2 If no argument is given, the new channel data will be stored in the first free channel buffer.
ACP i(;aaaa)	Assemble CP-list with number i. Range i: 1-63. aaaa is the element-name from which on the list must be modified or assembled.
ADC aaaa	ADd Channel with element-name aaaa to all samples of the file opened with the OPF command and ask for the values.
ADF (DEV:)(XXXXXX.YYY)	ADd File with filename XXXXXX and extension YYY to the file opened with the OPF-command. If no device is given, the same device as by the OPF-command will be taken. If only the device is given, the same filename and extension as by the OPF-command will be taken.
ADS XXXXXXXXXX	ADd Sample with identification XXXXXXXXXX to the file opened with the OPF-command. The first 20 characters will be stored on disk.
AJB i	Assemble JoB i (i= 1-63).
AMB i	Assemble Monitor-Buffer i. Range i : 1-63.
AML i	Assemble Moduli-List with number i. Range i: 1-63.
ALL i	Assemble Limits-List with number i. Range i: 1-63.

ALP i

Assemble LP-list with number i. Range i: 1-63.

AMP i

* Assemble Measuring Program i (i= 1-63).

AMS i

Assemble Moduli-Set with number i. Range i: 1-63.

ANM i

Assemble long-NaMes starting with position i in the name-list.

ARC i

Assemble RC-set with number i. Range i: 1-31.

ASC i (J)

* Philips sample changer: Measure with the Automatic Sample Changer up to and including tray i (i=0-165).
If an argument J (1-999) has been given, the tray and position number in the output reports will be replaced by this sequence number. This sequence number will be raised by one for each new sample loaded from the sample changer. If the same sample has been loaded for the second or next time after a RCS command, it will set the same sequence number as used during the first measurement.

ASP

Assemble System-Parameters. With this command the terminal-type (PR , VT, GT) can be defined as well as two concentration-output-devices or listing-output- devices and the maximum number of characters to be printed on each device (devices: TT,LP,RT,SY and PP). Furthermore the outlay of the user ident groups can be defined (see chapter 5).

BMD

* Batch MoDe. After a measurement without the sample changer the cap will not be opened. Sample turret positions 1, 2, 3 and 4 may be used for loading samples.
With the sample changer all available positions will be loaded.

CAL aaaa(,r)

Calculate the ALpha of element aaaa. If no real value has been given, no start value for the alpha will be assumed (start value = 0); otherwise value r will be denoted as start value.

CAN xxi

* Calibrate the ANgle of channel xxi (for xxi see the ACH command). The system will ask for the measuring time (TIME: 1.0 :=) and the range (RANGE: .20 :=). The calibration sample must have been loaded and transported to the measuring position before. A stepscan will be executed from channelset angle -.5*RANGE degree to channelset angle +.5*RANGE degree with a stepsize of .005 degree. The measuring time per step is t seconds. The default value for t is 1 sec and the default value for the RANGE is .2 degree. The allowed values for the RANGE are .10 - .63 in steps of .01. The angle belonging to the maximum intensity (averaged over 3 adjacent points) is the new channel set angle. The new peak angle is not stored in the channel set if the question 'SAVE: YE :=' is answered with N.

CBT aaaa(,r)

Calculate the BeTa of element aaaa. Rest as CAL.

CCD i aaaa

Correct Concentration-Data of element aaaa in sample i. For DJ- and RH-model.

CCD i

Correct Concentration-Data of regression element in sample i. For LP-model.

CEB

Change Equivalent Background

CHC i aaaa

CHange Concentration-data. Of the data to be changed, the sample number is i, and the element name is aaaa.

CHI i aaaa

CHange Intensity-data. Rest as CHC.

CID i

Correct Intensity-Data of regression element in sample i. For RH- and DJ-model.

CID i aaaa

Correct Intensity-Data of regression element aaaa in sample i. For LP-model.

CLF — CLose the File opened by the OPF-command.

CMD — * Continuous MoDe. If the type of measurement is not direct ratio, the cap will be opened if the new sample is in the measuring position. If sample changer is connected, an old sample may be unloaded and the next sample will be loaded during a measurement. Only sample turret positions 2 and 4 can be used in this mode.
If manual, after loading a new sample,the cap can be closed by means of a /C.

COM text — Set second output device on and print the text on the second output device and on the operators terminal.

COL a — COLlimator a, a= F (fine) or C (coarse).

CPB — * Clear ParameterBank. This command will erase the parameterbank (CH, MP, JB).

CST (i) (J) — Calculate STatistics. The default values for i is 1, and for J equal to the nr. of samples in the file. If only i has been given the range is: i- nr. of samples in the file.

CTS x s — ConTinuous Scan to angle x with speed s degrees/min. For x see the SLS command; s= .25, .5, 1, 2, 4, 8, 16 or 32 degrees 2 theta per minute.

DCF (i) — Delete sample Changer File.
If no argument given, all samples will be deleted from the file. If one uses an argument, only the indicated batch of samples will be deleted from the file. The operator must then also remove the batch of samples from the sample changer. If one batch of samples has been measured, it is automatically removed from the file and the sequence numbers of all remaining groups are lowered by 1.

DCP i — Delete CP-list with number i. Range i:1-63.

DET a — DETector a, a= F, S or FS.

DJB i — Delete JoB i (i= 1-63).

DLC aaaa — DeLete Channel. In all samples in the file opened with the OPF-command, the concernins channel aaaa will be deleted from the file.

DLL i — Delete Limits-List with number i. Range i: 1-63.

DLP i — Delete LP-list with number i. Range i: 1-63.

DLS i — DeLete Sample. Delete sample i from the file opened with the OPF-command.

DMB i — Delete Monitor-Buffer i. Range i : 1-63.

DML i — Delete ML-list with number i. Range i : 1-63.

DMP i — * Delete Measuring Program i (i see DMP).

DMS i — Delete MS-list with number i. Range i : 1-63.

DPB — * Dump ParameterBank. The contents of the parameterbank will be dumped to the terminal in hexadecimal format 70 characters (=35 memory locations) per line. If a cassette or papertape punch has been connected to the terminal it is possible to make a tape which can be loaded with the RPB command. The parameterbank from the microprocessor will be dumped to diskette with the same filename as the current databank. The file extension however will be .PBK

DRC i — Delete RC-set i. Range i : 1-31.

DSA i(,J) — Delete SAmple. If two arguments have been given, delete sample from number i till and including sample number J. If no argument given, all samples will be deleted.

EJB — End of a JoB. This is the last command in a joblist.

END — Terminates the X14D-software program.

FAL aaaa(,r) — Fix the ALpha of element aaaa. If no real value has been given, the old value of the alpha will be fixed; if a real value r has been given, the alpha will be given the r value.

FBT aaaa(,r) — Fix the BeTa of element aaaa. Rest as FAL.

FLT a — FiLTer a, a= Y(ES) or N(O). Yes means filter in.

FRT — Fetch Reference Tray.

FTM — Finish TransMission ; resets RTM- and STM-commands.

IAB — Interrupt After this Batch.
After this command the measurement of the present batch from the Herzog automatic sample changer will be finished, but the measurement of the next batch will not be started.

ISA (i) (J) — Include SAmple again. If one argument is given, include that sample; if two arguments are given, include samples starting from i till and including sample J; if no argument given, include all samples again.

KVM i J — KV and Ma setting i and J. The allowed KV settings i are 0, 25 (5) KVMAX (60 or 100) and the allowed mA settings are 0 10 (5) 80. If i and/or J is 0, the manual setting of the generator control panel will be selected. An error message will be generated if the product i*J is above the maximum x-ray tube power or i>max. voltage (60/100) (see XRT command). If the kV is 25, no mA above 65 is accepted.

LDB (DEV:)XXXXXX

Load DataBank with name XXXXXX into memory. In assembly-mode new added data to the databank in memory will be added to XXXXXX (name given with the last LDB-command) or in case the LDB-command has not yet been given, to file FW1400. Default device: SY0. The file-name must always be given.

LDM i

* Load monitor into turret position i (i=1-3).

LTU i

* Load sample TUrret position i with a sample from the Sample Changer (i=1-4).

LWL i

LoWer Level i, i= 0-99.

MAN

MANual mode, all input from the operator goes to micro-processor and all data from microprocessor will be printed until the command AUT is given as response to C=.

MCF

Measure samples according to the sample Changer File, using the Herzog automatic sample changer.

MPY i

* MultiPlY the scaler/timer settings in SMX or SMM measurements with a factor i. For i are allowed: 1, 2, 4, 10, 20 and 40. The selected values for the preset time and the preset counts will temporarely be multiplied by i. The resulting preset counts value will be rounded to the next selectable value. The resulting preset time and/or preset counts value will not go above 999.9 sec and/or 5*10**7 counts if the original selected value was not 0 (infinite).

MSK i

MaSK i, i=1 or 2.

MTY i

* Philips sample changer : Move the TraY in such a way that position i is in the loading position (i= 1-6).
Herzog sample changer : See below: 'Measurements with the Herzog sample changer'.

NPI

No Printing of gross Intensities (reset of PIN-command)

NRE — Next REgression element. Start with next regression.

NRL i — Number of lines on the operators VDU is i (i= 0 or 6-100). If no VDU is used, i should be 0. Used with the PCH command.

OPF (DEV:)XXXXXX.YYY — OPen File with filename XXXXXX and extension YYY. If no device given, SY1: will be the default device.

ORD i — ORDe i, i= 1-2.

PCD (i) (J) — Print Concentration-Data. Same as PCI-command, but only the concentrations will be printed. Nett intensities will be printed if the CP-number was 0.

PCF (i) — Print sample Changer File.
This command will print or display the contents of the sample changer file on the operators terminal. It gives a survey of the workload of the sample changer. The batches which are already processed are automatically removed from the file, so these are not showed. This command may be given during the measurements.

PCH (xxi) — * Print the CHannel parameters of the xxi channel. For the definition of xxi see ACH. If no argument has been given, all channel parameters will be printed, but the maximum numbers of lines on a screen (see NRL command) will be taken into account.

PCI (i) (J) — Print Concentration- and Intensity-data. If no argument the concentratation and intensities of all samples will be printed. If i given, only the concentrations and intensities of sample i will be printed. If two arguments given, the concentrations and intensities of the sample startins with sample i till and including sample J will be printed.

PCP i — Print CP-list with number i. Range i : 1-63.

PCS iEJ — Preset Counts Setting i*10**J to the preset counts buffer (i=0,1,2,5 and J= 4,5,6,7). The value i=0 means preset counts not used (infinite). The preset time will be made equal to 999.9 sec (maximum value).

PCS ssss (,dat) — Print Concentration data from samples having a specified strins ssss in the identification and evtl. a specified date.
The % character is used as a 'do not care' character. The format of the date id day(1-31), month(1-12) and year (70-99).

PHD (xxi)

* Pulse Height Distribution curve. After this command, the system will ask for the window w (WINDOW: 5 :=) and the time t (TIME: 1.0 :=). The default value for the window w is 5 and the range is 1-20 %. The default value for the measuring time is 1 second and the range is 0-999.9. If t=0 the recorder will be used and no data are printed on the terminal.

PID (i) (J)

Print Intensity-Data. Same as PCI-command, but only the intensities will be printed.

PIN

Print gross INtensities.

PJB i

* Print JoB i (i= 1-63).

PJF

Print Job-file opened with OPF-command before.

PLL i

Print Limits-List with number i. Range i : 1-63.

PLP i

Print LP-list with number i. Range i : 1-63.

PLT

PLoT program.
This command plots the results of the regression-analysis. The command will ask for the definition of the y- and x-axis and if required for the non-regression-element (if x-axis = 3). In the case x=2 and y=1,2 or 3, the line D+ER can be drawn on the screen after the points have been plotted by typing the letter L followed by carriage-return. If the letter G followed by carriage return is given, a grid will be drawn. If another plot is required, simply type-in carriage-return, after which the data on the screen will be erased and the PLT-command can be given again.

The PLT-command can only be given if there is a graphical terminal allocated.

PLS (arg)

PLot Spectrum. This command plots the contents of a stepscan in a Job-file. If no argument has been given, all stepscans in a file will be consequetively plotted. If the argument is an integer, the stepscan with that sequencenumber will be plotted only. If the argument is an element-name, the first scan in the file with that element-name will be plotted only.
The stepscan can be plotted in various modes and with various y-scales; therefore see the description of subroutine PLSCOM-PLOTSP resp. PLSHP and PLOTHP.
Stepscans with less than 3 points are skipped; if the X-axis values are changed by the user in such a way that only 2 or less points remain in the stepscan, an error-message INVALID will be generated and the program asks for new X-axis values.

PMB i

Print Monitor-Buffer i. Range i : 1-63.

PML i

Print ML-list with number i. Range 1 : 1-63.

PMM

Print Memory Map of databank in memory.

PMP i

* Print Measuring Program i (i see AMP).

PMS i

Print MS-list with number i. Range i : 1-63.

PNM

Print long-NaMes from name-list.

PPB (a)

* Print ParameterBank contents.
If an argument i has been given:
a=C Print channel names.
a=M Print only MP nrs. and free space.
a=J Print only JOB nrs. and free space.
a=F Print only free space.
If no argument has been given, all these data will be printed in sequence C, M, J, F.

PRC (i)

Print RC-set(s). If no argument has been given, all RC-sets will be printed; with argument, only the RC-set with the argument number will be printed. Range i : 1-31.

PRL (i) (J)

PRint List of calculated concentrations. If one argument given, print from that sample number on; if two arguments present, print from sample number i till and including sample number J; if no argument, all samples will be printed.

PSI (i) (J)

Print Sample-Identification. Same as PCI-command, but only the sample-identifications will be printed.

PSP

Print System-Parameters.

PTC t iEJ

This is a combination of the commands PTS and PCS. The contents of the preset time buffer will be made equal to t and iEJ goes to the preset counts buffer.

PTS t

Preset Time Setting t to preset time buffer. The contents of the preset counts buffer will be made 5E7 counts (maximum preset count value). The allowed values of t are 0-999.9 sec in steps of .1 sec. The value 0 means no preset time (infinite).

PTY i

Program TraY i. Define measuring-programs for samples in the tray, independently from the tray-card.

PWR i k

* Defines the maximum X-ray tube PoWeR as i kWatts (i= 0.0-3.0). The second argument k defines the maximum kV of the generator (60 or 100 kV).

RCF (aaaa)

Reset Correction Factor. Resets the CAL-command; if, no element name given, all correction factors will be reset; if an element-name is given, only the correction factor for that element will be reset.

RCJ i

* ReCycle Job i times (i as in RCM).

RCM i

* ReCycle Measuring program i times (i= 0-127, 0 means infinite). The recycle number will be printed in the output report. The maximum printed value will be 255.

RCS i

* ReCycle Sample changer i times (i as in RCM).

RES	* RESet the commands MPY, RCM, RCJ, RCS and ASC. Individual reset is possible with the commands MPY 1, RCM 1, RCJ 1 and RCS 1.
RMS iEJ	RateMeter Setting i*10**J counts/sec. The allowed values are: i= 0, 1, 2, 5, and J= 2, 3, 4, 5. Automatic range is indicated by i=0.
RPB	* Read ParameterBank made with the DPB command.
RTM	Request TransMission to second concentration output device. After the output of data on the first concentration output device, it is requested whether the output should be transmitted to the second concentration output device.
SAR i	Start Automatically Recalibration for measuring program i.
SCH xxib	Set parameters of CHannel xxib in the spectrometer. For the definition of xxi see ACH command. The symbol b is a space (main angle), a + sign (main angle + +offset) or a - sign (main angle - -offset).
SCT	Start Counter/Timer.
SJB i (I)	Start JoB i (i= 1-63). After the start there will be printed JB followed by the job number i. If the last character is an "I", the computer will ask for the sample identification (20 characters).
SLF x	SLew Fast to angle x (x see SLS) and make an angle approach loop.
SLP i	Sample turret position i to Loading Position. Position i will go to the loading position and the cap will go up.
SLS x	SLew Slow to angle x (0<= x<= 147.505 degrees) without an angle approach loop.

SMA i(,J,k)

Start Measuring and calculate Apparent concentrations with MP-number(s) i(,J,k). Rest as SMX-command.

SMM i,(J),(k)

* Start Monitor Measurement with program i,J,k (i,J,k= 1-63). If the RCM command has been given, the measurement will be recycled.

SMP i

* Sample to Measuring Position i, i= 1-4. The cap will be closed and sample turret i will go to the measuring position.

SMR i

Start Manual Recalibration for measuring program i. The WDD-command must have been given first and the CP-list must be mentioned in the LP-list as otherwise an error message will be printed.

(SMX) (i) (J) (k)

* Philips sample changer or no sample changer at all : Start a measurement with program(s) i (J and k). The allowed values for i-k are 1-63. If the command is only a carriage return, a new SMX measurement will be started with the same measuring programnumber(s) as given for the last sample(s). If the system is in batch mode (see BMD command) the system will ask for the sample turret positions to be loaded: SAMPLES= 1 (m) (n) (o) (I) The allowed values for l-o are 1-4. If the last character is an I, the system will ask for the (alpha-numeric) sample identifications of maximum 12 characters and bring the corresponding sample turret position to the loading position. Closing with I is not allowed in a SMX command in a Joblist. If the system is in continuous mode (see CMD command), the system will not ask for the sample turret positions, but it will ask for the sample identification for turret position 2 or 4.

SOT a

Second Output Terminal, a=Y or N.

SPN x

* SPiNner on (x=Y) or off(x=N).

SPR i(,J,k)	Start Prepare Regression. Measure and write regression-intensities with MP number(s) i(,J,k) to disk. The WDD-command must have been given first as otherwise an error-message will be printed. Rest as SMX-command.
SRA	Start Regression-Analysis.
SRI	Start Regression-Input. The maximum number of samples is 99 and the maximum number of elements to load is 1200/nr of samples. The maximum number of elements which can be loaded is never greater than 20.
SRP (yy) (tt)	Start Regression-analysis and Print intermediate results. yy is the number of iterations and tt is the tolerance.
SRR i	Save Regression Results in CP-list i.
SRT	Store Reference Tray.
SSM ss	Single Step Mode. The stepping motor will make a single step of size ss (for the allowed values of ss see STS command) after a carriage return of the operator. This step will be made in the direction of a higher angle. The steps will go to lower angles if once a minus sign has been given before the carriage return. If thereafter a plus sign is given before the carriage return; the steps will be made again in the direction of the higher angles. If instead of a + or - sign a new value is given; this new value will be used as new step size. The angle limits .0 and 147.505 may be passed in this command, to check the micro switches.
SSR i	Start Semi-automatically Recalibration for measuring program i. The WDD-command must have been given first as otherwise an error message will be printed.
STM	Start TransMission to second concentration output device. After this command all output will always be printed on both concentration output devices.
STS x ss	STep Scan to angle x with stepsize ss. For the value of x see SLS command; ss is .005 - .635 in steps of .005 degrees.

ACF (i)

Assemble sample Changer File.
If no argument is given, the new sample(s) will be added behind the samples which are already in the file. If an argument is given, it is possible to change the data of batch i which is already in the file.
After the ACF command the system will ask for the measuring program number to be used for the batch. If the spectrometer is not busy it will check whether this measuring program exists in the uP parameterbank. Next it will ask for the identification of the batch and for the number of samples in this batch (0-999, 0 means unknown). If the answer for the number of samples is a carriage return only, the batch size is determined by the first empty position detected behind this batch. Finally it will ask for the sequence number (0-999) of the first sample in the batch. If the answer is only a carriage return, the first sample will get sequence number 1 if it is a batch of more then 1 sample and no sequence number will be added if it is a batch of just 1 sample.
It is also possible to introduce a monitor measurement to update a monitor buffer. In that case the letter M must be added after the input of the measuring program number (just before the carriage return, separated by a space or comma from the measuring program number). The system will then ask whether the monitor will be available in one of the sample turret positions. If the answer is NO it will ask for the external monitor position (0-7). If the answer is 0, the monitor will be loaded from the sample changer as is the case with unknown samples. If the answer is 1-7 the monitor will be loaded from the Herzog reference tray.
If an external monitor position has been indicated, the system will load the monitor always in sample turret position 1, so this must be indicated in the applied MP list, else an error-message is given.
The operator has also the responsibility that position 1 is free; in batch mode there must be sufficient empty positions in the sample changer so that the whole batch preceding the monitor can be unloaded!!!
The ACF command may also be given during the execution of the measurements of the samples in the SC file, so it is possible to load and identify new samples, while the sample changer is already in use.

STY (i)

* Philips sample changer : Search TraY i, i= 0-165. Position 1 of tray i will be moved to the loading position of the sample changer. If no argument has been given, the next tray (pos.1) will be moved to the loading position. Herzog sample changer : See below: "Measurements with the Herzog sample changer".

TST (C)x, aaaa (,llll) Test command to read data (x=R), to write data (x=W) or to start a program on address aaaa (x=E). If x=R reading starts in location aaaa and llll values are read and printed, the default value for llll is 1. If x=W the new value(s) should be given behind aaaa. All values in this command are hexadecimal. If x is preceded by C, the command is continuously executed until the carriage return key is pressed.

ULM i

* Unload monitor from turret position i (i=1-3).

UPL i

UPper Level i, i= 0-99 (0 means window infinite). If UPL<=LWL the window is 0.

UTU i

* Unload sample TUrret position i to the Sample Changer (i=1-4).

WDB (DEV:)XXXXXX

Write DataBank from memory to disk with name XXXXXX. Default device: SY0. The file-name must be given.

WDD (DEV:)(XXXXXX)

Write Data from memory to Disk with filename XXXXXX. The default device is SY1. Default name is the same name as before has been given.

XTL i

set XTaL i, i= 1-6.

2. DATA PROCESSING

The output data from the basic (microprocessor controlled) version of the PW 1400 will show accumulated counts and measurement time for each element in the sample measuring program(s). This section of the manual will describe the X14 software and the operations possible using the intensity/time data, when a PDP11 computer is installed. Using these procedures an output showing the chemical concentration of the elements in samples is possible.

The operation and description of optional items, such as sample changers, helium flushing system, etc., are shown in paragraph 3.

A PW 1400/00 Spectrometer supplied with a PDP11/04 Minicomputer system, will comprise:
- The PW 1400 Spectrometer with microprocessor and software programs in PROMs (programmable read only memories), and parameter bank capacity in RAMs (random access memories).
- A DEC PDP11, connected via the PW 1400 input/output interface.
- A RX01 flexible (floppy) disc unit with two stations (drive units).
- Two flexible (floppy) discs with the X14D software programs, (generation discs) – see below.
- One or more peripheral devices (see paragraph 3.4) with the main terminal capable of typing command information and reading out analysis data (normally hard copy). The main terminal is connected to the PDP11.

```
X14D-GENERATION-DISKETTE  VERSION 2.0
15-OCT-79                 4022 151 84621
DISKETTE 1/2  50HZ/RT/HP2648A-HP2649C

PROPERTY OF
N.V. PHILIPS' GLOEILAMPENFABRIEKEN
EINDHOVEN - NEDERLAND
```

Disc 1/2 containing the 60Hz version of the X14D software, for use with PDP11 with HP 2648A or HP 2649C Graphics terminal.

```
X14D-GENERATION-DISKETTE  VERSION 2.0
15-OCT-79                 4022 151 84631
DISKETTE 2/2                60HZ/RT/VT55

PROPERTY OF
N.V. PHILIPS' GLOEILAMPENFABRIEKEN
EINDHOVEN - NEDERLAND
```

Disc $^2/_2$ containing the 60Hz version of the X14D software, for use with a DEC VT 55 graphics terminal.

System disc labels

If the required 50 or 60Hz version software is not on the same disc as the program for the graphics terminal to be used, place disc 2/2 in staion 0 (DX0) and disc 1/2 instation 1 (DX1). Put the Boot /INIT switch to Boot and when the bootstrap input is complete type " @ 60Hz" or " @ VT55" @ 60Hz is input for a 60Hz clock with a HP 2648A terminal, and @ VT55 is input when a VT55 graphics terminal is used with 50Hz software. The disc in station 1 is now the "system" disc, and should be copied immediately.

2.1. DESCRIPTION OF THE SOFTWARE PACKAGE

The X14 software program to be used is on a flexible disc, normally loaded into the left-hand station (labelled 0) of the two disc drive units. A "files" disc containing measurement results and other data is loaded in the right-hand station.

Software notes

Sample analysis will use the microprocessor software described in paragraph 1, in addition to the computer software described in this paragraph. Therefore, the operation notes on pages 1.3 to 1.5 should be studied in conjunction with these notes before using the spectrometer system.

Copy the delivered X14D software programs onto a flexible disc (for daily use), and keep the system (master) disc in a safe place - refer to paragraph 2.7.2.

Commands used in the X14 software are similar to the microprocessor commands, and the comments at the start of paragraph 1.2 will apply, e.g. commands are three letter abbreviations, etc.

Correction of a letter(s) is possible by operating the Decwriter DELETE key (per incorrect character), or a line of input by operating the CONTROL U key, both provided that a carriage return has not been given.

Databank and parameters banks

Parameter bank is the name given to the information contained in the **microprocessor** memory (RAM), and consists of channel sets (CH), measurement program lists (MP), and job lists (JB), see the microprocessor description in paragraph 1. It is used for spectrometer control. Keyword: spectrometer operation.

Databank is the name given to the information contained in the **minicomputer** memory, and consists of link programs (LP), countrate correction sets (RC), calculation parameters (CP), monitor buffer list (MB), moduli list (ML), moduli sets (MS), names list (NM), and limits list (LL). It is used in the data handling. Keyword: Calculations (and results reporting).

Databank assembly

The system disc delivered contains a databank designated PW1400DBK , which is automatically loaded when the system is started and initiated, see paragraph 2.1.2. The parameters which are input by the X14 software (ALP, ARC, ACP, etc.) go to the computer and are immediately stored in the disc databank. It is recommended that a "files" disc be used to contain all databanks and parameter banks for routine use.

Place an initiated flexible disc (see paragraph 2.1.2.) in disc drive 1 and give the command WDR DX1: xxxxxx which copies the empty databank PW 1400 DBK to the files disc under the name xxxxxx. Now load that databank again to the memory, using the command LDB DX1: xxxxxx. All future list assembly will now be stored in the databank file xxxxxx in the files disc in disc drive 1, until another file is loaded. The PMM command can be given to show which databank has been loaded, and to readout details of its contents.

Writing and loading of databanks

Databank files are identified with a six character identification, plus a file type identification (the letters DBK). The file type identification is automatically added when the WDB and LDB commands are given, so a databank can be loaded from a disc using the command LDB xxxxxx, where xxxxxx is the identification name of the databank file.

The PMM command will give a readout of the databank name, and the contents of the loaded databank.

The loaded databank can be written to disc, that is copied, using the command WDB xxxxxx, where xxxxxx is the identification name on the disc for the databank file, e.g. LOALST (for low alloy steels). If a databank file with that name already exists on the disc, the file is overwritten with the input data and this enables the updating of databank files.

The WDB and LDB commands are executed on the disc loaded in station 0 (system disc), unless otherwise specified, i.e. the default value is 0. If the disc in station 1 has to be used, it is selected by giving DX1: xxxxxx as a command argument, e.g. LDB DX1: xxxxxx.

Parameter banks

The assembly of parameter bank information (ACH, AMP, AJB) proceeds directly with the microprocessor, and data are stored in a RAM. Hence, the input data are not written automatically to disc, but the complete parameter bank can be written to disc by the operators command DPB. This command causes the whole contents of the parameter bank to be written to the disc into a parameter bank file. An identification name for this file is not specified when the DPB command is given, and the parameter bank data will be written to a file on the disc from which the databank is loaded, and will have the same file name identification as the data-bank identification. The parameter bank data will have a file type identification PBK to distinguish it from the databank data.

A parameter bank file can be read into the RAM again, using the RPB command, after loading the corresponding databank (which has the same name as the parameter bank data).

Files identification

Databank	– 6 characters, plus DBK	(file type identification)	e.g.	LOALST.DBK
Parameter bank	– 6 characters, plus PBK	(file type identification)	e.g.	LOALST.PBK
Concentrations file	– 6 characters, plus Cxx	(file type identification)	e.g.	STEELS.C50
Regression file	– 6 characters, plus Rxx	(file type identification)	e.g.	STEELS.R50
Recalibration file	– 6 characters, plus Bxx	(file type identification)	e.g.	STEELS.B50
Job file	– 6 characters, plus yyz	(file type identification)	e.g.	SPECTR.34A

where xx is the MP number
yy is the job list number
z is a letter from A to Z corresponding to the number of times that SJByy command has been given, i.e. 1 to 26 measurements.

2.1.1. Software organisation

The assembly of channel sets, measurement parameter lists, and job lists is exactly as described in paragraph 1.5. These data are stored in the parameter bank of the microprocessor (RAM), and must be read out separately to any data stored in the computer databank. It is possible to load new measurement data to the parameter bank via an X14 link program (LP list). This links the measurement parameters to correction and calculation para-meters which will be stored in the computer databank.

The computer software programs are on the system flexible disc, and the programs are organised in modules, as below:

- Assembly (AS), to build up, change, or delete the information in databank and parameter bank e.g. link program, correction and calculation parameters, and other lists.
- Analysis (AN), to start calibration procedures, measurement and calculation of concentrations, and related functions.
- Initiation and a few reset procedures.
- Update (UP) to manipulate the contents of the files stored in the "files" disc.
- Hardware test, see the Service Manual.
- Regression (RG), to calculate the instrument and sample dependent constants, using calibration values from a range of standard samples.

Note that all assembly and most measurement commands used in the microprocessor software, paragraph 1.2, can also be used in the AUTomatic mode, i.e. given from the computer terminal with asterisk (*) dialog.

The survey of commands listed in paragraph 2.2. is generally as the module listing show above, but the grouping is functional and the particular command may not be in the headed software module, or it may appear twice in the survey. Note that a number of microprocessor commands (parameter setting, goniometer position, etc.) can only be given in the MANual mode i.e. using the microprocessor C = dialog.
In this case the computer is not used except to transmit data between the microprocessor and the computer terminal.

Initiation of the XR14 software is simple and is described in paragraph 2.1.2. After initiation any of the commands listed in paragraph 2.2. can be given. As mentioned above, the MAN command is given to revert to microprocessor (C=) only dialog.

The two station disc unit will normally be loaded with two flexible discs:

- a **system disc** in station 0, containing the X14D programs.
- a **files disc** in station 1, which can contain one or more databank files (including parameter bank data), regression, recalibration and measurement results, etc.

A typical files disc readout is shown in figure 2.1A.

```
.DIR DX1:
 23-Mar-79
DB1400.DBK      5 22-Mar-79       DB1400.PBK      3 21-Mar-79
STEELS.R50      3 22-Mar-79       STEELS.B50      3 22-Mar-79
STEELS.C50      3 22-Mar-79
 5 Files, 17 Blocks
 463 Free blocks
```

Fig. 2.1A. Readout of files disc contents.

The following terminology is used with the X14D software, which may appear in some readouts:

Disc	— Flexible (floppy) disc (disk) mounted in the disc drive unit in station 0 or 1.
Block	— A sub-division of the disc, there are 480 blocks per disc. A block contains 256 words.
File	— A set of records covering a **whole** number of blocks, i.e. a file can be one or more blocks.
Record	— A sub-division of a file. Each record contains data of one sample (C, R and B files). The length of the record is variable (in words), and depends on the number of channels measured.
Word	— 16 bits.

2.1.2. Computer and disc operation

The PDP11 Computer and RX01 disc drive unit are housed in a separate cabinet, see figures 2.1B. and 2.1C.

Fig. 2.1B. PDP11/04 Computer system

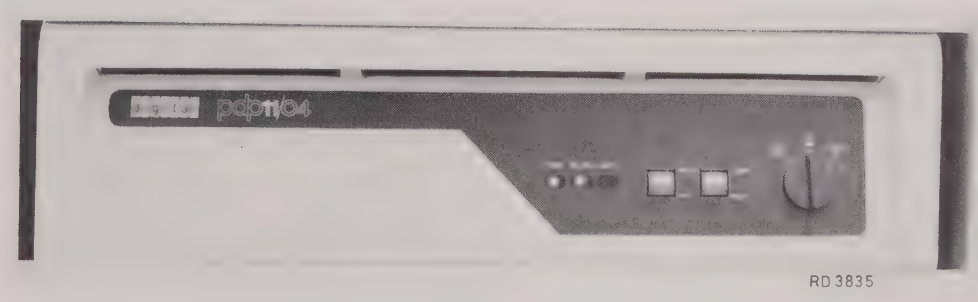


Fig. 2.1C. Computer control panel.

Modes of the software dialog

There are three modes of conversation:

– "Dot"	•	using the DEC RT11 monitor software
– "Asterisk"	*	using the X14-D software
– "C ="	C=	using the PW 1400 microprocessor software.

Refer to the RT11 Manual for the "dot" mode description, and to paragraph 1 for the "C = " mode description.

Start up and initiation

When the PW1400 system is switched on by the generator MAINS I push-button, the computer will be operational if the PDP11 control panel knob is set to DC ON.
The RUN and DC ON lamps should be lit.

Note that during switch on and switch off the loading flaps of the two disc drive units should be open if they are loaded with a floppy disc. This will prevent any switching transients from affecting the data on the discs.

On the PDP11 control panel momentarily operate the BOOT key to INIT. The PDP11 internal program will run and type four groups of numbers as shown in figure 2.1D.

Ensure that the system disc with the X14-D program is loaded into the left-hand disc drive station (DX0), and the drive unit flap is closed. The disc is inserted with the label on top and to the front . Note that the master disc (X14-D programs) delivered with the system should be copied, and the copy used for system operation – see paragraph 2.7.

Type DX, and this will cause the initial program on the system disc to be read into the computer. The computer will then output the system parameters, and the time and date which are already in the memory. The system parameters are described below, and the date and time can be updated as shown in figure 2.1D.

```
000000 030434 001074 000030        Typical output from PDP11 internal program
@DX                                Read in initial program from the system disc
RT-11SJ (S)V03B-00C

.SET USR NOSWAP

.TIME 09:00:00

.DATE 15-OCT-79

.INSTALL RT:

.ASS RT: 4

.SET RT CR

.SET RT LC
                                   ← Input new date and time, if required
.R PW1400

X14D-002.0                         Ready for asterisk dialog

*
```

Fig. 2.1D. Initial program loading.

Note that a number of the readout examples shown later in this paragraph were obtained using the P851 computer system, and the format of date and time is different, for example 01-MAR-79 09:00 is printed as 01-03-1979 09.00.

While the dialog is still in the dot mode the system programs can be started by typing "R (space) PW 1400 carriage return" as above.

The initiation program will run, and when complete will output "X14D-xxx", and an asterisk to indicate that X14-D commands can now be input. The xxx designation in the software identification shows the serial number of the system disc, see figure 2.1E. This figure also shows the print memory map command PMM, which outputs a listing of the list data stored in the memory, and the remaining free space – in this case the memory is empty.

.R PW1400	Run initiation program
X14D-000	Program accepted, and system disc identification is printed.
* PMM	Print memory map (note * dialog).
SY0:PW1400	Note databank name PW 1400
LF 0	No link programs stored
FREE SPACE 2986 WORDS	Total space in memory for list assembly etc.
*	Ready for input of next command.

Fig. 2.1E. Initiation and print memory map.

In the asterisk mode the commands listed in paragraph 2.2. can be given, and note that these include most of the commands described in paragraph 1, also see pages 1.13 to 1.16. The command MAN will select to C= dialog (microprocessor only), and the command AUT will revert to * dialog from C=.

To revert to the "dot" mode (RT-11) give the END command. This may be necessary if time and date are to be changed.

Switching off

Open the doors of the disc drive units 0 and 1, if a disc is loaded, before switching off the system (MAINS 0 operated).

Initiating a files disc

A "files" disc is used to record the analysis programs and sample measurement results for specified sets of samples, possibly including regression analysis results. This files disc must "initiated" before it can be used to record files data i.e. certain marks and, if required, monitor programs must be pre-recorded on the disc. This is done in the "dot" mode, and it is recommended that the RT11 manual is studied. Two methods are possible:

1. With the X14-D system disc in station 0, and a new (or other) disc in station 1, copy the systems disc by giving "@ COPY" (in the dot mode), where @ is the Decwriter upper case 2. The X14D files will overwrite any previous data if a used disc is in station 1.
   Now delete the following files (DEL DX1: xxxxxx.xxx):
   PW 1400.SAY COPY.COM
   PW 1400.DBK X14DY1.HED
   SYSPAR.DAT
   @COPY will require files COPU. COM and COPYTX.LST.
   The remaining programs on the "files" disc take up some space, and if this space is required for other files, and if a copy of the "files" disc is not required, use the INIT routine.
2. The INIT routine places marks at the beginning of the new disc, and erases all existing data. The system disc must be in station 0.
   Give the command INIT/BAD BLOCKS DX1: (for the disc in station 1), and answer the dialog "init are you sure? " with "Y". Note that BAD BLOCKS can be left out if error detection is not required.

Readout of files on a disc

A readout of the file identifications from the system disc, or a files disc, is obtained when the directory command is given in the "dot" mode. The disc station must also be specified as below:

```
.DIR DX0:      Give the directory contents of the disc in station 0
 29-Oct-79
SWAP   .SYS     24 11-Mar-78        DXMNSJ.SYS     61 07-Jun-79
TT     .SYS      2 07-Jun-79        LP     .SYS     2 30-Dec-78
RT     .SYS      2 07-Jun-79        DIR    .SAV    17 11-Mar-78
DUP    .SAV     21 24-Mar-78        PIP    .SAV    16 11-Mar-78
RESORC.SAV     12 11-Mar-78        PW1400.SAV   275 15-Oct-79
X14D20.HED      1 22-Aug-79        STARTS.COM     1 15-Oct-79
PW1400.DBK      3 21-Dec-78        SYSPAR.DAT     1 18-Sep-79
COPY   .COM     1 06-Sep-79
 15 Files, 439 Blocks
 41 Free blocks
```

Readout of the system disc contents

```
.DIR DX1:      Directory of disc in station 1
 23-Mar-79
DB1400.DBK      5 22-Mar-79        DB1400.PBK     3 22-Mar-79
STEELS.R50      3 22-Mar-79        STEELS.B50     3 22-Mar-79
 4 Files, 14 Blocks
 466 Free blocks
```

Typical readout of a files disc contents, as figure 2.1A.

Selection of input and output peripherals

When the system is first used, or when the type of terminal is changed, the system parameters must be defined by typing the command ASP, see figure 2.1F. The terminal type used to input data and the output device must be defined, plus an optional second output device.

Input and output can be on the same device (output device = TT) or on separate devices (output device = RT). The latter is called **remote terminal**; for example if data is input from a VDU (terminal type = VT) a printer can be used to receive the output data (output device = RT) in which case the VDU will not display this output data.

In addition an optional **second** output device (output only) can be connected to the computer. This allows e.g. results reporting at two different locations. The commands RTM,STM and FTM apply for the transmission to this second output device.

Note that another output device can be connected to the **spectrometer (microprocessor)** interface, but this will only readout counts and time data (not concentrations, etc.), and the commands SOT and COM will apply when the system is in the MANual mode only.

The sample identification (20 characters max.) can be subdivided into separate fields up to 6. The length of each field must be input separately, but the total number of characters must not exceed 20.

Note that the ASP command input data are stored on the system disc in station 0 in file DX0:SYSPAR.DAT.

When the ASP command is given the following inputs can be given to define the type of peripheral and its characteristics:

Terminal type	: PR = printer (PC 1409) : VT = VDU (P817) : GT = graphical terminal
Output devices	: TT = terminal, i.e. the terminal type defined above is used for output : LP = line printer : RT = remote terminal (see above) : PP = papertape punch

```
* FSP                                  Print (existing) system parameters.
TERMINAL TYPE= VT                      Video display unit used as input terminal
LINES/SCREEN =  24                     24 lines per page — see paragraph 1.5.2.

CONCENTRATION AND LISTING OUTPUT DEVICES :
 1 = TT   WIDTH =  80                  Output to main terminal (VDU as above)
 2 = LP   WIDTH = 132                  Output to line printer — if required, see paragraph 2.4.9.

NR  IDTEXT  WIDTH                      see ASP input
 1 IDENT      20

* ASP                                  ASP given to change main terminal
TERMINAL TYPE= VT    := PR             Printer keyboard used for input device
CONCENTRATION AND LISTING OUTPUT DEVICES :
 1 = TT    :=                          Printer also used to record output.
WIDTH =  80 :=
 2 = LP    :=
WIDTH = 132 :=

NR OF IDENT FIELDS = 1 :=              Maximum of 6 fields, with total of 20 characters
FIELD WIDTH 1 = 20 :=                  Input number of characters in field 1
TEXT1 =IDENT     :=                    Input identification text of field 1


* FSP                                  Print system parameters
TERMINAL TYPE= PR

CONCENTRATION AND LISTING OUTPUT DEVICES :
 1 = TT   WIDTH =  80
 2 = LP   WIDTH = 132

NR  IDTEXT  WIDTH
 1 IDENT      20

*
```

Fig. 2.1F. System parameters (peripherals) selection.

2.1.3. *Concentration calculation*

The output from the spectrometer (microprocessor) to the computer consists of a listing of the intensity (counts) and measurement time for each element line (channel set) which was included in the measurement program. The output of counts will have been corrected for dead time and pulse contraction or pulse shift.

The computer will first convert the count and time output to a countrate r'' (counts per second).

Background and line overlap correction

The measured countrate will invariably contain two background components, one which is constant (shown as B), and another which will vary between different sample matrices and is practically straight (see figure 2.3C).

A first and second background correction can be applied according to the formula:

$$r' = r'' - l_1 r_1'' - l_2 r_2'' - B$$

Where:

r'	= Net countrate corrected for background
r''	= Gross countrate
l_1	= Correction factor (L1) for channel 1 (CHL1)
r_1''	= Countrate with channel 1 (CHL1)
l_2, $r''2$	= Correction factor and countrate of channel 2
B	= Fixed background countrate

Note — A background channel (denoted by a + or —) can be subtracted when input during the RC set assembly, e.g. if CHL1 = MO + or MO — , but RC input is not always necessary, see 2.3.2.

The final spectral correction for line overlap can then be made by using the corrected countrates (r') in the second part of the equation:

$$r = r' - l_3 r_3' - l_4 r_4'$$

Where:

r	= Net countrate corrected for background and line overlap
l_3	= Correction factor (L3) for channel 3 (CHL3)
r_3'	= Countrate with channel 3 (CHL3)
$l_4 r_4'$	= Correction factor and countrate of channel 4

The net countrate after correction is thus:

$$r = r'' - l_1 r_1'' - l_2 r_2'' - l_3 r_3' - l_4 r_4' - B \text{ counts per second}$$

Ratio calculation

1. External ratio calculation is used to relate countrates from different elements in a sample to the countrates of the same elements from a stable reference specimen (instrument monitor). This method will eliminate the effect of residual long term drift (if any) on the analysis results. The ratio is calculated from:

$$R_i' = (r_i)_x / (r_i)_m$$

Where:

R'	= External countrate ratio
r	= Net element countrate (counts per second)
x	= Denotes unknown sample
m	= Denotes reference sample (monitor)

Monitor measurements can be performed in the buffer ratio mode or the direct ratio mode, but ratio calculation procedures are similar.

2. Internal ratio calculation uses the measurement of an element line in the unknown sample, or the known reflected tube lines. The equation is now:

$$R_i = (r_i/r_j)_x$$

Where: R = Internal ratio
r = Net element countrate (cps) or countrate ratio
x = Denotes unknown sample

This internal ratio technique can be used for spiking or standard addition, using elements added to the unknown samples, or it can be used to correct for changes in the dilution ratio, sample size or shape, absorption coefficient, etc.

Concentration mathematical models

The concentration C can be calculated from C = D + ER, where R can be either the directly measured countrate or the normalised ratio, and corrected as above. The constants D and E for each element are instrument dependent, and they can be easily updated periodically for high order measurement accuracy. This linear equation assumes that there are no, or negligible, matrix effects, and is only appropriate in applications where element concentrations are reasonably equal between samples. In many applications this is not the case, and more complex mathematical models are used to include corrections for matrix effects, see figure 2.1G. Three calculation models are included in the PW1400 software, but note that figure 2.1F is typical for model DJ only.

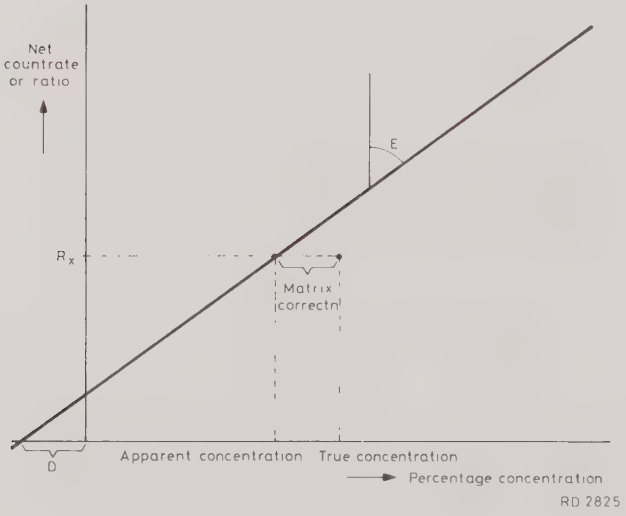


Figure 2.1G. Calibration curve to determine chemical concentration.

Model LP – intensity based correction

The intensity based correction formula is:

$$C_i = (D_i + E_i \,.\, R_i)\ (1 + \Sigma \alpha_{ij}\, R_i/100)$$

This gives the concentration of element i, compensated for the matrix effect due to element j.
In this equation, D_i and E_i are element and instrument dependent constants which can be measured and stored in the computer memory.
The model is known as the Lucas-Tooth-Pyne model and it is suitable for analysis of samples with small elemental concentration ranges. Because the correction is based on the countrate of the interfering element, correction factors can also be derived for those elements for which the concentration is not known.

Model DJ — concentration based correction

The concentration based correction model proposed by de Jongh, in which fundamental influence coefficients (alphas) can be applied, is expressed in the formula:

$$C_i = (D_i + E_i \,.\, R_i)\,(1 + \Sigma a_{ij} \,.\, C_j/100)$$

The corrections are based on the concentrations of the interfering elements, and the calculation uses a set of simultaneous equations.

This formula resembles the Lachance-Traill model, but includes corrections for self-absorption effects. It is extensively used and has proved successful for most applications.

The influence coefficients (alphas) are constant for a given type of sample analysis, and a given X-ray tube type and spectrometer type combination. The alphas can be calculated in the regression routine using the regression data (regression calculated alphas or experimental alphas). On the other hand Philips can provide tables with alpha values (for any combination of specified sample matrix, and spectrometer and tube type), derived from physical data (theoretical alphas). The application of theoretical alphas is extremely useful if only a small number of standard samples are available and, therefore, cannot be calculated from the regression data.

Theoretical and experimental alphas can also be used together.

Model RH — concentration based correction

The correction model proposed by Rasberry-Heinrich is expressed by the following equation:

$$C_i = (D_i + E_i \,.\, R_i)\,(1 + \sum_j \alpha_{ij} \,.\, C_j/100 + \sum_k \beta_{ik}\, C_k/100[1 + C_i/100]^{-1})$$

The object of the second correction term is to provide a better fit over an extra wide range of compositions. The software now includes the calculation of beta in the regression program, but theoretical values are not available.

2.1.4. Extended calculations.

From the concentrations results, extended calculations can be made e.g. normalisation, correction for sample dillution, and moduli calculations.
Normalisation involves the linear correction of the concentrations to bring the sum of all concentrations to a predefined value. Each concentration is there by multiplied by the normalisation factor $NF = X/\Sigma Ci$ (in which X is the predefined value). Refer to 2.4.5. **Correction for sample dillution** involves the multiplication of all concentrations with the dillution factor DF which is the final sample weight divided by the initial sample weight. Refer to 2.4.5. **Moduli calculations** involve the calculation of a linear function of the concentration (s) in the sample, which can generally be expressed as:

$$M = \frac{X_1C_1 \pm X_2C_2 \pm \text{etc}}{X_3C_3 \pm X_4C_4 \pm \text{etc}}$$

Refer to 2.3.6.

2.2. SOFTWARE COMMANDS

The X14 software commands also include a number of commands previously described in paragraph 1.2, such as assembly and analysis commands. The notes which preface paragraph 1.2. also apply, that is:
- Commands are three letter abbreviations (except stop commands).
- Commands can be followed by one or more arguments, each separated by a space (or comma).
- Commands must be terminated by a carriage return, after the last argument is given, and then the required action is initiated.
- The command listing shows the range of an argument thus: SMX i, where i must be a number from 1 to 63.
- Optional arguments are shown between brackets thus: SMX i (j) (k), means that the number for i is mandatory, but j and k are only given if required.
- In addition note that default values are shown, i.e. if an argument is not given the system will apply a given value.

A number of **PW 1400 commands** do not appear in the X14 software, and can only be given in the manual (microprocessor) mode — give command MAN. For convenience these commands are listed below:
AUT, COL, COM, CTS, DET, FLT, LWL, MSK, NRL, ORD, PCS, PTC, PTS, RMS, SCH, SCT, SLF, SLS, SOT, SSM, STS, UPL and XTL.

The software programs are on a disc, and are organised in modules are listed below, but selection of a module on a disc is not necessary.
- Analysis module
- Assembly module
- Regression module
- Update module

The following survey of commands is intended to be functional, and does not necessarily relate to the order of assembly in the software modules.

Assembly

COMMAND/ARGUMENT	MEANING
ACH	Assemble a new channel. The order of the readout of channel data is the same order in which the channels sets are assembled.
ACH x(x)(i)	Assemble or change the parameters of channel xxi. The first x of a channel name must be a letter, and can be followed by an optional letter and/or a number. Up to 63 channels can be assembled. See figure 1.3A.
PCH	Print all channel data, in blocks of 5 channels, see figure 1.3B.
PCH xxi	Print the parameters of the specified channel.
PWR i k	The maximum values of the power (i) and voltage (k) of the H.T. generator are defined, where i = 0 to 3 (kilowatts) in 0.1 steps, and k = 60 or 100 (kilovolts) — for the PW 1730/10 or the PW 1732/10 generator.
ANM i	Assemble compound names, starting with combination number i. Up to 63 element/compounds can be assembled in the names list. Terminate the list assembly by a slash (/). Type DL to delete an element/compound combination.
PNM	Print element/compound names list.
AMP i	Assemble a measurement parameters list number i, where i = 1 to 63. See figure 1.3C.
PMP i	Print the measurement parameter list number i.
DMP i	Delete the measurement parameter list number i from the memory.

COMMAND/ARGUMENT	MEANING
AJB i	Assemble a job measurement program number i, where i = 1 to 63. Refer to paragraph 1.3.3.
DJB i	Delete the job measurement program number i from the memory.
■ EJB	End of a job measurement program to terminate J = input (revert to C =)

■ Means that the command can be assembled in a job list (AJB), and the job measurement commences from the SJB command or by selection from a sample changer tray identification card.

▲ Means that the command can be included in a job list, but the list cannot be selected from a sample changer card.

ALP i	Assemble a link program number i, where i = 1 to 63. To be linked with MP list i.
DLP i	Delete link program i.
PLP i	Print link program i.
AMB i	Assemble monitor buffer list i, where i = 1 to 63.
DMB i	Delete monitor buffer list i.
PMB i	Print monitor buffer list i.
ARC i	Assemble countrate correction set i, where i = 1 to 31.
DRC i	Delete countrate correction set i.
PRC i	Print countrate correction set i.
ACP i (xxi)	Assemble calculation parameters list i, where i = 1 to 63, from element name xxi onwards, if required. Default value for xxi in an existing CP list is the first channel.
DCP i	Delete calculation parameter list i.
PCP i	Print calculation parameter list i.
AML i	Assemble moduli list i, where i = 1 to 63.
DML i	Delete moduli list i.
PML i	Print moduli list i.
ASM i	Assemble moduli set i, where i = 1 to 63.
DMS i	Delete moduli set i.
PMS i	Print moduli set i.
ALL i	Assemble limits list (concentration limit) i, where i = 1 to 63.
DLL i	Delete limits list i.
PLL i	Print limits list i.
PMM	Print a memory map, of the contents of the databank.
WDB (DXi:)xxxxxx	Write a databank having the file name xxxxxx, from the memory to the disc in station i, where i = 0 or 1. Default value of i is 0 (left-hand station).
LDB (DXi:)xxxxxx	Load the databank with the file name xxxxxx from the disc station i, into the memory, where i = 0 or 1 and default value is 0. Assembly data added to the databank will also be input to the LDB file, or to PW1400 if the LDB command has not been given.
END	Revert to dot mode

COMMAND/ARGUMENT	MEANING
PPB	Print the contents of the parameter bank, to show the channel names, numbers of the MP lists and JB lists, and the remaining free space (in words) in the memory.
PPB a	Print the specified part of the parameter bank, where a = C to show list of channels a = M for MP list numbers a = J for job list numbers a = F for free space only.
DPB	Dump the parameter bank data onto disc, to preserve a record if the parameter bank is to be cleared. The RPB command is used to read the data back into the memory.
RPB	Read the data from disc into the parmeter bank.
CPB	Clear all data from the parameter bank.
• ASP	Assemble the system parameters to define input and output devices, and line widths. Default values are printer (main terminal — input and output).
• PSP	Print the system parameters.

Analysis

COMMAND/ARGUMENT	MEANING
■ SMX i (j)(k)	Start measuring unknown samples, using measuring parameter list (MP) i, and j and k if required. i (j and k) = 1 to 63. Give a space between arguments. See also paragraph 1.4.
SMA i (j)(k)	Start measurement and calculate apparent concentrations, using MP lists i, (j) and (k), otherwise as SMX.
■ SMM i (j)(k)	Start measuring monitor sample, using measuring program i, j, k. i, j, k = 1 to 63.
SPR i (j)(k)	Start prepare regression, using MP lists i, (j) and (k). First give the WDD command (or an error message will be printed), and the measured intensities will be written to the defined disc file.
i (j)(k)	Start measurement using the previously input measurement mode.
c.r.	Start measurement using the previously input measurement mode and MP lists.
SJB i (I)	Start measurement using the job program i. i = 1 to 63, with sample identification if required.

One of the following recalibration commands can be given:

SMR i	Start manual recalibration using MP list i.
SSR i	Start semi-automatic recalibration using MP list i.
SAR i	Start automatic recalibration using MP list i.

The following PWR and SPN commands can be given to set initial system conditions, and are only reset to another value.

SPN a	Set spinner to condition a, where a = Y (yes = on) or a = N (no = spinner off). The spinner will not run (a=Y) until the sample measurement commences.

When the PW1400 is switched on or reset the spinner is set to on. The SPINNER warning lamp is lit when the spinner is not running.

■ KVM i j	Set the H.T. generator output toi kV and j mA, where: i=25 to 100kV in 5 kV steps, and j = 10 to 80 mA in 5 mA steps. To reduce generator output values to minimum before switching off.

The following commands can be given before the start measurement commands above, to modify or extend the measurement program.

PIN	Print gross intensity measurement results in addition to the concentrations output. Reset by NPI.
NPI	No printing of gross intensities (concentrations only).
CMD	Continuous mode measurement. The cap is open during the measurement of a previously loaded sample, and this allows the continuous loading and measurement of samples. Turret positions 2 and 4 are used. Refer to paragraph 1.4.5.
/C	In continuous mode cap closes and sample passes through airlock.
BMD	Batch mode measurement. Samples are loaded into turret positions 1 to 4, before measurement, and the cap remains closed until all results are printed.
RCM i	Recycle the measurement program i times given before a start measurement command. i = 0 to 127. 0 means infinity. Refer to paragraph 1.4.6.
RCJ i	Recycle job program i times (before SJB). i = 0 to 127. Refer to paragraph 1.4.8.
MPY i	Multiply the preset time and preset count values i times, where i = in the MP lists. Refer to paragraph 1.4.6
RES	Resets all RCM, RCJ, MPY, ASC and RCS commands. The individual commands are also effectively reset when i = 1, except ASC.

The following STM and RTM commands can be given before the start measurement command to output results to a second peripheral device connected to the computer (via its interface). They do not apply to any optional output device connected to the second **microprocessor** interface, which uses the SOT and COM commands.

STM	Start transmission to a second output device connected to the computer, to print all measurment results on concentration and listing output devices 1 and 2 as specified in ASP.
RTM	Request transmission to a second output device connected to the computer. The sample measurements results are printed on concentration and listing output device 1 and the operator can decide

	whether to repeat the readout to the second device, effected by giving a carriage return.
FTM	Finish transmission, resets the STM and RTM command

The following commands can be given in addition to the above sample measurement commands.

■ CAN xxi	Calibrate the angle of channel xxi, where xxi is the name of the channel - see ACH command. Refer to paragraph 1.4.10.
PHD (xxi)	Pulse height distribution readout of the channel xxi, where xxi is the name of the channel see ACH command. Refer to paragraph 1.4.11. and 2.4.10.
SLP i	Turret sample position i to loading position, where i = 1 to 4. Cap is open.
▲ SMP i	Turret sample position i to measuring position, where i = 1 to 4. Cap is closed.
▲ LDM i	Load monitor sample in turret position i, where i = 1 to 3 (BMD), 1 and 3 (CMD).
▲ ULM i	Unload monitor sample in turret position i, where i = 1 to 3. Cap is open.
WDD (DXi:)(xxxxxx)	Write measurement results to the disc in (disc drive) station i, with a file name xxxxxx, where i = 0 or 1. Default disc station value is 1. Default file name is the one previously given.
NDD	No data to disc, to reset WDD.
MAN	Manual mode, to switch the microprocessor control (C=) software control. Reset to computer control (X - 14 * mode) by command AUT.

The following commands can be used when a sample changer is installed, refer to paragraph 3.

▲ LTU i	Load sample from the changer into turret position i, where i = 1 to 4.
▲ UTU i	Unload sample from turret position i to the changer, where i = 1 to 4.
▲ STY i	Search for tray number i = 1 to 165 (loaded on tray program card). The changer will search until position 1 of the selected tray number i is in position ready to be loaded into the spectrometer.
▲ MTY i	Move the tray to bring the sample position i ready for loading, where i = 1 to 6.
▲ FRT	Fetch the tray of reference samples, stored in the PW 1500/00 six-position changer, with reference tray option PW 1505/00. Refer to paragraph 3.1.
▲ SRT	Store the reference tray (PW 1500/00 with reference tray option PW 1505/00).
ASC i (j)	Automatic sample changer to be used for the measurement of samples up to, and including tray i, where i = 1 to 165. The optional argument j is an identification number from 0 to 999, which is raised by 1 for each new sample loading.
RCS i	Recycle sample changer measurements i times. i = as RCM command.

PTY i	Programmed tray i, where i = 1 to 165, can have a separate measurement program and sample identification for each sample.

Stop commands

/	Stop measurement program (or other action) immediately slash **and** carriage return given.
/S	Stop the scaler/timer operation and print the results. If a further measurement is programmed this will start after the printout of the results.
/M	Stop after the completion of the measuring program of the samples. Used to interrupt a recycling program, or to interrupt a measurement routine using the automatic sample changer. The original recycling command is not reset.
/T	Stop after the complete measurement of samples in a tray in the loading position of the automatic sample changer. The next start measurement command will commence measurement of the samples in the next tray.

COMMAND/ARGUMENT	MEANING
Regression	
SPR i (j) (k)	Start prepare regression - see Analysis commands
ACD (i)	Assemble concentration data starting with sample number i, where i = 1 to 63. Default value is 1. See also Update commands.
SRI	Start regression input of intensity and concentration values from disc file opened with OPF command. Maximum number of samples is 99, the maximum number of elements is 20 or 1200/number of samples.
SRA	Start regression analysis.
PRL (i) (j)	Print list of calculated concentrations for all samples (no arguments) or for sample (i), or for samples (i) to (j).
DSA i (j)	Delete sample i from regression calculation, or samples i to j.
ISA (i) (j)	Insert all samples (no arguments) in the calculation, or sample (i), or samples (i) to (j).
CCD i	Correct concentration data of regression element in sample i, for **LP calculation models.**
CCD i xxi	Correct concentration data of element xxi in sample i, for **DJ and RH calculation models.**
CID i	Correct intensity data of regression element in sample i, for **DJ and RH calculation model.**
CID i xxi	Correct intensity data of regression element xxi in sample i, for **LP calculation model.**
FAL xxi (r)	Fix the alpha of element xxi to the value (r). Default value of r is the previously input or calculated value.
FBT xxi (r)	Fix the beta of element xxi to the value r. Default value of r is the previously calculated value.
CAL xxi (r)	Calculate the alpha of element xxi, with a starting value of (r). Default value of r is zero.
CBT xxi (r)	Calculate the beta of element xxi, with a starting value of (r). Default value of r is zero.
RCF (xxi)	Reset correction factor of element (xxi), to reset the alpha or beta values input from CAL, FAL, CBT and FBT commands. If the element name is not given all correction factors are reset to zero.
CEB	Change equivalent background.
SRR i	Save the regression results in the CP list i. If i is given for a new CP list an identification name can be input.
NRE	Next regression element, the next element name for regression analysis can be input.
SRP (i) (tt)	Start regression analysis and print intermediate results, where (i) is the number of iterations and (tt) is the tolerance.
PLT	Plot the results of a regression analysis

COMMAND/ARGUMENT	MEANING
Update	
OPF (DXi:)xxxxxx.yyy	Open file with identification xxxxxx and extension yyy on the disc loaded in station i, where i = 0 or 1. Default value for i is 1 (right-hand station).
ADF (DXi:)(xxxxxx.yyy)	Add a file with identification (xxxxxx) and extension (yyy) on the disc loaded in station i, where i = 0 or 1. If the first argument is not given the disc chosen is that given by the OPF command. The default value for the file is that chosen by the OPF command.
CLF	Close the file opened by the OPF command.
ACD (i)	Assemble concentration data, starting from sample (i) onwards. Default value for i is 1.
ADS x	Add a sample x concentrations/intensities to the file opened by the OPF command. Sample identification x can be up to 20 characters.
DLS i	Delete the sample number i details from the file opened by OPF.
ADC xxi	Add a channel with element name xxi to all samples of the file opened by the OPF command. Concentration/intensity values must be input.
DLC xxi	Delete the channel data for element name xxi, for all samples, from the file opened by OPF.
PSI (i) (j)	Print the sample identifications, for all samples (no arguments), or for samples (i) to (j), or for sample (i).
PID (i) (j)	Print the intensity data for all samples (no arguments), or for samples (i) to (j), or for sample (i).
PCD (i) (j)	Print the concentration data for all samples, for samples (i) to (j), or for sample (i).
PCI (i) (j)	Print concentration and intensity values for all samples, for samples (i) to (j), or for sample (i).
PJF	Print the job file from the file previously opened by OPF.
CHI i xxi	Change the intensity data for sample number i, of the element xxi.
CHC i xxi	Change the concentration data for sample number i, of the element xxi.
CST (i) (j)	Calculate the statistics for all samples in the file (no arguments), for samples (i) to (j), or for sample (i) to the maximum number in the file.
PLS (i) (xxi)	Plot a spectrum of a step scan in an opened job file, with an integer i or channel xxi as an optional argument, see paragraph 2.4.7.

2.2.1. Error messages

Error messages can be generated by the microprocessor software programs, or by the computer software. The microprocessor messages can be recognised as they are prefixed by two asterisks (**), refer to the listing in paragraph 1.2.1. (pages 1-11, 1-12).

The computer messages are prefixed by three asterisks (***), and are listed below. This listing shows a letter prefix which is **not printed** but is included to indicate the severity of the error, thus:

f — means that the error is fatal, and further action is not possible. Repeat command or input after corrective action, or type correct information.
r — means recoverable error, the command is not interrupted but the correct input must be given.
w — means a warning, the command input is not interrupted but check that the data or conditions are corrected later (e.g. before analysis).

f:*** GIVE FIRST WDD COMMAND	SPR command given, but WDD must be input first.
r:*** INVALID	Incorrect answer in list assembly.
f:*** INVALID ARGUMENT	Command argument is not correct repeat command with proper arguments.
f:*** INVALID COMMAND	Command not correct, repeat with proper input.
r:*** INVALID, CORRECT VALUE :=	Argument or input value not correct.
f:*** UNKNOWN LIST	List to be changed/deleted or printed is not in the memory.
f:*** UNKNOWN FILE	File does not exist in the selected disc.
f:*** UNKNOWN CHANNEL	Channel data does not exist in the selected file or list.
f:*** NO SPACE IN DATABANK	Databank full, no space for new lists.
f:*** TOO MANY ELEMENTS IN CP-LIST	More than 63 elements in the CP list
f:*** .. IS NO JOB-FILE	File opened is not a job file.
f:*** .. IS JOB-FILE	File opened is a job file.
f:*** ERROR D1	Hardware error during a write action to the disc.
f:*** ERROR D2	Hardware error during a read action from the disc.

f: *** ERROR D3	Disc driver error, or disc not loaded.
f: *** ERROR D4	Expected data is not on the disc.
f: *** ERROR D5	Disc overflow.
f: *** ERROR D6	Contents of the file with concentration results does not agree with the current data in the MP list.
f: *** ERROR D7	Unexpected end of file.
f: *** ERROR D8	Channel data cannot be deleted. The last-file on the disc can be deleted by the computer command DLF.
f: *** ERROR E1	Spectrometer is busy.
w: *** ERROR EE AAAA BBBB CCCC	No convergence of the concentration calculations after 10 iterations, and the elements which do not converge are AAAA BBBB CCCC.
w: *** ERROR EF	Insufficient space in monitor buffer for new element.
w: *** ERROR LL	Requested limits list (LL) is not in the memory.
w: *** ERROR OV	Too many elements (> 63) in the results buffer (due to the manual input of intensities and/or concentrations or to the calculated element by difference).
w: *** ERROR R4 FOR ELMNT AAAA	Arithmetic error, or measured intensity is zero, for element AAAA.
w: *** NO DATABANK IN MEMORY	Requested databank is not in the memory.
f: *** NO FILE OPEN, GIVE OPF COMMAND	Before using the update procedures open the required disc file with the OPF command.
r: *** INVALID SAMPLE NR, NR OF SAMPLES=	Sample number input is too high, type the correct number
f: *** UNKNOWN ELEMENT	Requested element is not known (name not input).
f: *** NO BETA ALLOWED IN THIS MODEL	Beta not allowed in calculation models DJ and LP.
r: *** INVALID, MAX NR OF COR'S=	The number of correction factors for the element is greater than 20.

f:*** NO REGRESSION DATA	Regression analysis has not commenced.
f:*** NO INTENSITIES IN THIS FILE	The file opened in the disc does not contain intensity data, for example as required in the regression analysis procedure.
f:*** MORE THAN 20 ELEMENTS	More than 20 elements requested with the SRI command.
f:*** INVALID MODEL IN CP-LIST	The calculation model used in a requested CP list does not agree with the model shown in the SRI command input.
w:*** MATRIX SINGULIER	Correlation in the concentration data.
W *** NO CONVERGENCE	No convergence in the regression analysis calculation.
W *** DISK OVERFLOW, GIVE CR AFTER MOUNTING NEW DISKETTE OR / AND CR IF NO NEW DISKETTE WILL BE MOUNTED	Disc full with data, mount a new initiated disc and c.r., or give a slash (/) and c.r. if a new disc will not be mounted.
F *** DUPLICATE CHANNEL-NAME	Input channel name already exists in the file.
w:*** SPECTROMETER OFF	Dialog not possible with the microprocessor, cable not connected or PW 1400 not switched on.
F *** INVALID CHARACTERS FROM SPECTROMETER	Invalid hexa-decimal characters, or too few characters, received from the spectrometer.
F *** ERROR TP	Error in the transmission to the microprocessor
F *** ERROR TR	Error in the transmission from the microprocessor.
w:*** ELEMENT AAAA NOT IN CP-LIST; NO RECALIBRATION	Element AAAA is not assembled in the CP list, therefore, recalibration for this element is not possible.
w:*** MONITORBUFFER .. DOES NOT EXIST	Monitor buffer list number . . has not been assembled.
W *** MONITORBUFFER .. IN LP LIST ... EMPTY	Element data of monitor buffer list, given in link program list, are not present, i.e. the monitor has not yet been measured.
f:*** MONITORBUFFER .. IN LP LIST .. UNKNOWN	The monitor buffer quoted in LP list number .... does not exist.
f:*** NO GRAPHICAL TERMINAL	Graphical terminal not selected (use ASP command), or not connected, when PLT command is given.
F *** LP-LIST .. UNKNOWN	LP list . . not assembled in the databank in the memory.
w:*** NO SYSTEM-PARAMETERS ON DISC 0	System parameter file on disc 0 not present. Assemble using the ASP command.

f:*** ERROR UP	Error in the communication with the microprocessor (UP).
f:*** CP-LIST IN LP-LIST .. UNKNOWN	A CP list is not given in LP list . .
f:*** MULTIPLE DEFINED FILENAMES	Two files added to each other by the ADF command have the same file names.
w:*** MODULUS-LIST .. NOT PRESENT	
w:*** IR-ELEMENTS NOT MEASURED	Internal ratio elements . . are not measured.
f:*** INVALID; GIVE FIRST DMB-COMMAND	Monitor buffer list already exists, delete with DMB.
w:*** UNKNOWN MODULI-SET(S): MS.. MS.. MS..	Moduli sets are not assembled.
f:*** ERROR BO	Overflow of microprocessor buffer.
w:*** MODULUS XX NOT CALCULATED; DENOMINATOR ZERO	Denominator of modulus is zero
w:*** .. UNKNOWN IN MODULUS SET ..	Element not measured.
f:*** WRONG NUMBER OF CHARACTERS FROM SPECTROMETER	
f:*** CONTINUOUS MODE NOT ALLOWEDFOR RECALIBRATION	Spectrometer must operate in the BATCH mode for recalibration.
f:*** ONLY 1 MP ALLOWED FOR RECALIBRATION	Chaining of MP lists is not allowed for recalibration.
f:*** FILE ALREADY EXISTS	SMR not allowed, recalibration file already exists.
w:*** TO CONTINUE STRIKE THE CARRIAGE-RETURN KEY	Given on VDU when page is full.
f:*** NO MONITORBUFFER IN LP-LIST	
f:*** NO CP-LIST IN LP-LIST ..	
w:*** TOO MANY CORRECTIONS	In regression the number of corrections is too high for samples, degree of freedom $\leqslant 0$

W *** TOO MANY CHANNELS	Number of channels for results output will exceed 63. Only the first 63 channels will be used.
R *** INVALID FIELDWIDTH	Sum of all field widths given in the ASP command input exceeds 20 characters, see paragraph 2.1.2.
R ALL FILES ..... A-Z USED *** GIVE WDD-COMMAND WITH NEW FILENAME	Given when more than 26 job measurements have been written to file. Further job measurement data must be written to disc with a new file name.
W *** RESULT(S) OUT OF RANGE	Measurement results are outside the limits defined by the limits list, see paragraph 2.3.7.
F *** OLD FILE IS NOT A DATABANK	
F *** FILE IS NOT A PARAMETERBANK	
F *** EMPTY FILE	
R *** NEW FILE EXISTS ALREADY	The file name already exists on the new disc to which a copy file command has been given.
F *** FILE STILL ASSIGNED	The file to be deleted is still assigned.

2.3. ASSEMBLING THE ANALYSIS PARAMETERS

Assume that the system parameters (ASP command) have been input — see paragraph 2.1.2., and if in doubt use the PSP command. Also ensure that the PWR command input has been given.
The channel sets, measurement parameters lists, and job lists (if required), are assembled using the microprocessor software. This operation is fully described in paragraph 1.3., but the main details will be listed below. The sets and lists can be assembled in the MANual mode (computer inactive), or in the AUTomatic mode using the X−14 software.

Channel set

A new channel set is assembled from the command ACH, or an existing set is changed using ACH xxi. A total of 63 sets can be stored in the parameter bank, and assembly dialog is as follows:

NAME : =	Channel element designation x (x) (i)
LINE : =	Element line identification (KA, KB, LA, LB, LG or MA)
FILT : =	Beam filter in (Y = yes) or out (N = no)
COLL : =	Collimator choice, F = fine or C = coarse
DET : =	Detector choice, F = flow, S = scintillation, or FS = both
XTAL : =	Selection of crystal changer position, 1 to 6
ORDE : =	Order of reflection, 1 or 2.
% UL : =	Upper level setting from 0 to 99.
% LL : =	Lower level setting from 0 to 99. Note — window is % UL minus % LL.
KV, MA : =	HT generator output setting, from 25 to 100 (kV) and from 10 to 80 (mA).
ANGL : =	Goniometer 2θ angle from 0^{o} to 147.000^{o}
−OFFSET : = +OFFSET : =	Angle offset from 0 to $5{,}10^{o}$ 2θ, if required as a measurement channel in the MP list.

The setting of the upper and lower levels can be determined by using a pulse height distribution, as described in paragraph 4.4.4.

Note that the assembly of channel sets is fully described in paragraph 1.3.1.

Measurement parameters list

The measurement parameters list is assembled from the command AMP i, where i = 1 to 63.
Note that each measurement of unknown samples can use up to three MP lists. The assembly dialog is as follows:

MASK : =	Select collimator mask 1 or 2.
ABS : =	Select absolute measurement, Y (c.r.) or N.
*BRAT : =	Select buffer ratio measurement, Y or N (c.r.)
*MOPS : =	Monitor sample turret position 1 to 3.
*MOMPY : =	Time and counts multiplier for monitor measurement.

The dialog marked * does not appear if ABS : = Y (c.r.).

CHAN PT PC	Listing of channel names and preset time and counts required in measurement program.

The assembly of MP lists is fully described in paragraph 1.3.2.

Job list

A job list can be assembled, as described in paragraph 1.3.3. The command switches to J = dialog, and when the list is assembled the command EJB must be given to revert to C= or asterisk dialog. It is not possible to change or print a job list, but the command DJB can be used to delete a selected list.

Measurement of samples, according to a specified job list, can commence from the command SJB, or from selection by the identification card in a sample changer tray. Note that selection from the changer tray is based on the fact that the job list number is not the same as any MP list number in the parameter bank.

Preparing the computer lists

The above lists, which are stored in the microprocessor parameter bank, will normally be assembled before any other lists. The assembly of parameters for countrate correction and for concentration calculation, etc., are fully described in the following paragraphs. They can only be assembled in the AUTomatic mode using the X 14 software, and the list and set assemblied are stored in the **databank.**

It is necessary that the link program has the same number as the associated MP list, and it is suggested that other associated lists also have the same number, e.g. CP, MB, ML and LL.

2.3.1. Link program

The link program connects a measuring parameters (MP) list, stored in the microprocessor parameter bank., to various sets and lists which are, or will be, stored in the computer databank. The list will also further confirm the mode of measurement (absolute/buffer ratio), and select the calculations to be performed to produce percentage concentrations readout. Typical list assemblies are shown in figure 2.3A, and the measurement using these lists is described in paragraph 2.4.
Note that the link program (LP) list number must be the same as the associated measuring program list, e.g. list LP10 is automatically linked to MP10.

A maximum of 63 link programs can be defined, and the assembly command ALP initiates the following dialog:

NEW LIST — This is only printed when the list has not been previously assembled.

NRCH = — 0 to 63.
Input is required to show the number of channels that require data manipulation e.g. ratio calculation, line overlap correction, etc.

OPTIONS = — 0 to 2, 5 to 10.
Type the number(s) of the option to apply to the analysis as follows:

0	= no option, reset of previously selected options.
1	= manual input of concentrations
2	= manual input of intensities
5	= normalisation to x% (x to be given later)
6	= print the sum of the concentration
7	= element by difference (sum x to be given later)
8	= diluted samples
9	= check for concentration limits
10	= print of element names only

A full explanation of the above options is given in paragraph 2.4.5.

MBNR = — 1 to 63 (0 if not used).
The number of the monitor buffer list must be defined, if monitor measurement using buffer ratio is required. If the MB list has not been assembled (see paragraph 2.3.4.) a warning will be typed, but dialog is not inhibited.

INT. RATIO = — NO (or c.r.) or YE

If the answer is yes (YE) a countrate ratio is calculated after measurement of a specified (internal) element. Up to three internal ratio elements can be defined by the additional dialog INT 1 = , etc., and the element (s) channel name must be input.
If the answer is NO the normal dialog continues as below.

CPNR =	1 to 63 (0 if not used) The number of the calculation parameters (CP) list must be specified. It is recommended that the CP list number is the same as the LP and MP list number.
MODLST =	1 to 63 (0 if not used) Specify the number of the moduli list, to be used for the calculation of moduli, e.g. cement. Refer to paragraph 2.3.6.
CHAN RC IR A	A listing from 1 up to the number defined by NRCH =, to allow individual selection of parameter lists, etc. for element channel, with input as follows (each separated by a space).
CHAN	The channel element name.
RC	The number of the countrate correction set. Give a space or comma (or c.r.) if correction is not required. Note that when RC = 0 the background correction is normal, that is, the channel peak intensity will have the background (one offset angle) subtracted, or the average background (+ or — offset) subtracted (if these background channels are included in the MP-list).
IR	This column is only printed when INT. RATIO = YE, and requires the input of the internal ratio element channel name, or a space or comma (or c.r.) if not to be used.
A	This column is only printed when monitor buffer measurement is selected (MBNR = 1 to 63), to allow the absolute measurement of some channels. Type Y for absolute measurement, or N or space, comma (or c.r.) ratio measurement.

The examples of link program assembly, which are shown on next page, are based upon an absolute measurement program for cement and a buffer ratio measurement program for steels:

```
* PMP 10

MP 10

MASK :  2
ABS  : YE

CHAN    PT    PC
FE      10   0E0
CA2     20   0E0
K        4   0E0
S       10   0E0
S+      10   0E0
SI      20   0E0
AL      20   0E0
MG2-    20   0E0
MG2     40   0E0
NA      40   0E0
NA+     20   0E0


*
```

```
* PMP 50

MP 50

MASK :  1
ABS  : NO
BRAT : YE
MOPS :  1
MOMPY:  2

CHAN    PT    PC
MO      10   0E0
MO+      2   0E0
NB      10   0E0
NI      20   0E0
MN      10   0E0
CR      20   0E0
TI       4   0E0
P2      10   0E0
P2+      4   0E0
S2-      4   0E0
S2      10   0E0
SI      20   0E0


*
```

Absolute measurement program for cement, with moduli calculation.

```
* ALP 10
NEW LIST
NRCH=    0 ;=
OPTION=   0 ;=
MBNR=   0 ;=
INT.RATIO= NO ;=
CPNR=   0 ;= 10
MODLST=   0 ;= 10
```

Assemble link program 10 (associated with MP10)
Not previously assembled
No channels that require special action
No options
No buffer ratio } Therefore absolute measurement
No internal ratio }
Calculation parameters list 10.
Moduli list 10, see figure 2.3G.

```
* PLP 10
LPNR= 10      NRCH=   0      CPNR= 10      MODLST= 10      MBNR=   0
OPTION=   0

*
```

Note that background subtraction is carried out automatically for S, Mg and Na, as for those elements also a background channel is measured (refer to PMP 10).

Buffer ratio measurement for steels, with line overlap correction for P and S.

```
* ALP 50
NEW LIST
NRCH=    0 ;= 2
OPTION=   0 ;=
MBNR=   0 ;= 50
*** MONITORBUFFER 50 DOES NOT EXIST
INT.RATIO= NO ;=
CPNR=   0 ;= 50
MODLST=   0 ;=

     CHAN RC   A
  1=        0   N   ;= P2  1
  2=        0   N   ;= S2  2
```

Assemble link program 50.

Note that only those elements are specified that require special action e.g. line overlap correction.

Monitor buffer list 50 to be used.
Warning only

No absolute measurement, but (buffer) ratio.
Line overlap correction sets, see fig. 2.3B.

```
* PLP 50
LPNR= 50      NRCH=   2      CPNR= 50      MODLST=   0      MBNR= 50
OPTION=   0

ELMNT P2    S2
RC      1     2
ABS     N     N

*
```

Fig. 2.3A. Assembly of link programs.

2.3.2. *Countrate correction set*

The countrate correction set will correct the measured countrate of an element, for any background and line overlap effects.

The countrate correction set is assembled from the command ARC i, where i - 1 to 31. The dialog is as follows; also refer to figure 2.3B.

BKGR = 0 to 32767
Fixed background countrate (counts per second) to be subtracted from channel using the RC set.

CHL1 = The channel name of a background channel.

L1 = −3.2767 to +3.2767.
A multiplying factor applied to the countrate measured for channel L1.

CHL2 =
L2 = As above, but for a second background channel

CHL3 = The channel name of a line overlap intefering element.

L3 = −3.2767 to +3.2767.
A multiplying factor applied to the countrate measured for channel L3.

CHL4 = As above, but for a second line overlap interfering element.
L4 =

```
* ARC 1
BKGR=     0  :=
CHL1=        := P2+
L1= 0.0000   := 1
CHL2=        :=
CHL3=        := MO
L3= 0.0000   := .00158
CHL4=        :=
```

Assemble countrate correction set number 1 (for P2)

Plus offset angle of channel P2

100% background subtracted from channel P2

Interfering peak due to molybdenum

Empirically determined line overlap factor

```
* ARC 2
BKGR=     0  :=
CHL1=        := S2-
L1= 0.0000   := 1
CHL2=        :=
CHL3=        := MO
L3= 0.0000   := .00541
CHL4=        :=
```

RC set number 2 (for S2)

Negative offset angle for 100% background subtraction

```
* PRC
```

Print all (two) RC sets.

```
NR    BKGR   CHL1     L1      CHL2     L2      CHL3     L3      CHL4     L4
 1       0   P2+    1.0000            0.0000  MO       0.0016           0.0000
 2       0   S2-    1.0000            0.0000  MO       0.0054           0.0000

*
```

Fig. 2.3B. Assembly of a countrate correction set.

Following the intensity measurement of an unknown sample, an intermediate countrate is calculated by subtracting the constant background (BKGR =) and up to two variable backgrounds for channels CHL1 CHL2. These two channels have correction factors L1 and L2. A final calculation is performed using the line overlap correction factors L3 and L4 for channels CHL3 and CHL4. The line overlap correction (if assembled at CHL3 and/or CHL4) uses the background corrected intensities. The final result gives the net element countrate.

The correction constants BKGR and L1 to L4 are usually determined by measuring typical samples using the manual control, see paragraph 1.4.9. Referring to figure 2.3C, it will be seen that some idea of the spectrum around the element peaks of interest is useful, for the samples to be analysed.

A constant background (R_B) is easily determined by measuring the countrate close to the peak of interest, see figure 2.3C(a). The value BKGR = R_B.

A sloping background can also be determined by making offset angle measurements on either side of the peak. Referring to figure 2.3C(b), the value of L1 = L2 = 0,5 to give a net countrate R, where:

$$R = R_p - 0{,}5\ R_1 - 0{,}5\ R_2$$

The values for R_1 and R_2 will be due to the inputs CHL1 and CHL2, as above.

The constants for line overlap can be determined graphically, as shown by figure 2.3C(c), or by measurement. With the graphical method, the line of the interfering element is interpolated (shown dotted), to give a value Rm at the 2θ angle of the element line.
Then L3 (or L4) = $(R_m - R_b)/(R_o - R_b)$.

The second method requires the measurement of a sample **that does not contain the element of interest,** i.e. the value Rp is now the same as Rm, and L3 = $(R_p - R_b)/(R_o - R_b)$

It is assumed that the level of the interfering peak will vary in the same proportion as the level at the position of the peak of interest, so that the countrate R = $(Rp - R_b) - (R_o - R_b)$ L3.
The value for R_o is due to the input CHL3 (or CHL4 for a second overlap peak).

A third method can be used which is based on the measurement of samples of known composition containing the interfering element in varying amounts.
For instance, L3 can be computed by solving three equations resulting from the measurement of 3 samples:

$$C_i = E\ [(R_i - b) - L3\ (RL_i - b)]$$

in which i = 1 to 3
C = concentration of element of interest
E = sensitivity constant
R = intensity of element of interest
b = background
L3 = line/overlap factor
RL = intensity of interfering element

From these three equations L3 can be calculated by substituting the other two unknowns E and b.

Note that an RC set does not have to be assembled for "normal" background subtraction (factor 1 if one offset channel is measured or factor 0,5 if two offset channels are measured with the element concerned).

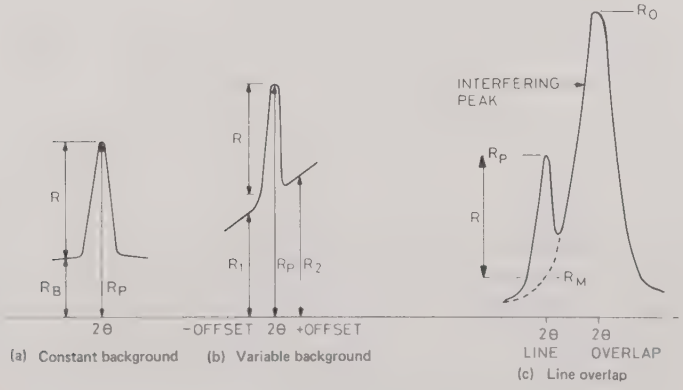


Fig. 2.3C. Determination of background and line overlap constants.

2.3.3. *Calculation parameters*

The calculation parameters list contains the D and E constants, and the alpha and beta values, as required, in order to calculate the chemical concentrations of elements in the sample for analysis. For each element, a D and E constant can be input, and for each interfering element an alpha value can also be input. When the Rasberry-Heinrich equation is selected a beta correction is also used.

The calculation parameter list (see figure 2.3D) is assembled from the command ACP i, where i = 1 to 63, but normally the list will be automatically assembled from the SRR command (save regression results) as a result of the regression analysis procedure, see paragraphs 2.5.3. and 2.8.2.

The ACP list dialog is as follows:

– NEW LIST	Is printed if the list has not been assembled previously.
– NAME=	Up to 30 characters can be given to identify the type of analysis, or measurement or calculation program. This identification can also be given during the regression analysis procedure from the **first** SRR command.
– MODEL = DJ : =	The model used for calculation must be defined, see paragraph 2.1.3., either De Jongh (DJ), or Rasberry-Heinrich (RH) or Lucas-Tooth-Pyne (LP).
– ELMNT = : =	The element channel designation, comprising up to two letters and an optional number (1 to 3). The order of the elements in the CP list determines the order in the readout.
– NDEC = 0 : =	Number of decimals to be used in the concentrations readout for this element, –1 to +5. If NDEC = –1 is selected the element concerned is not printed out in the concentrations readout.
– NCEL = 0 : =	The number of correction element (maximum 20) for which alpha (and beta) values will be input.
D = 0.00000 : = E = 0.00000 : =	The values (intercept and slope) used for calculation of apparent concentration are given. If values are not known let D = 0 and E = 1, in which case the concentration calculation will be in kilo-counts per second.
ELMNT ALPHA	For models DJ and LP. The element channel designation of the interfering, or correcting element is given and the alpha value. The input is repeated for each of the correcting elements (given by NCEL =).
ELMNT CORRECTION A/B	(For model RH). The element channel designation is given as above, and the correction factor must be defined whether it is an alpha (type A) or beta (type B) value.

The list assembly then continues with the request for the next set of element correction factors (from ELMNT = above) and the list assembly is terminated by a slash (/).

Note that the maximum number of matrix corrections which can be used in a CP list is 189, e.g. 15 elements each with 12 alphas.

```
* ACP 55                                   Assemble CP list 55.
NEW LIST
NAME =                                                  := LOW ALLOY STEEL
MODEL=   DJ :=                             De Jongh calculation model.

ELMNT=       := SI                         Element channel
NDEC=    3 := 2                            Number of decimals in readout.
NCEL=    0 := 8                            Number of correcting elements.
D=     0.00000 := -.00732                  Intercept of calibration line
E=     0.00000 := 1.08351                  Inverse slope

    ELMNT      ALPHA
 1=      ,     0.00000  := SI  ,794
 2=      ,     0.00000  := V  -,335
 3=      ,     0.00000  := CR -,189
 4=      ,     0.00000  := MN -,112        Interelement alpha correction factors
 5=      ,     0.00000  := CO  ,128
 6=      ,     0.00000  := NI  ,271
 7=      ,     0.00000  := NB -,383
 8=      ,     0.00000  := MO -,338

ELMNT=       := MN                         Next element
NDEC=    3 := 2
NCEL=    0 := 8
D=     0.00000 := -.01472
E=     0.00000 := .43862

    ELMNT      ALPHA
```

Continued for all elements to be used.

Fig. 2.3D. Assembly of calculation parameters list.

2.3.4. *Monitor buffer list*

The monitor buffer list serves to reserve space in the databank for the results of the measurement of a monitor sample, for a defined number of channels.

The monitor buffer list is assembled from the command AMB i, where i = 1 to 63. The MB list can be used by more than one LP list, and it can be updated by different SMM (start monitor measurement) programs. Thus, it is possible to create a monitor buffer for universal use.

The list requires only one input; see figure 2.3E:

NRCH = Number of channels for monitor sample measurement

```
* AMB 50                                   Assemble monitor buffer list 50.
NEW LIST
NRCH=    0 := 9                            Number of channels for measurement in monitor sample.
```

Fig. 2.3E. Assemble monitor buffer list.

2.3.5. *Names (compounds) list*

The names list is used to print a conveniently recognisable name in the measurements results readout, instead of the element channel name input in the MP/LP lists. Up to six characters can be used to describe the element name, and will normally be an element compound name (moduli), such as AL203 (Al_2O_3) in place of AL which appears in the MP/LP lists.

Assembly of the list (element/compound names) is initiated with the command ANMi , where i is the list number of the first combination to be assembled or changed. Up to 63 combinations can be assembled in the list.

Only one set of input is required, see figure 2.3F.

ELM, COMPOUND — The element input is the element name given in the ACH, MP and LP lists, i.e. xxi, or in the moduli set AMS, i.e. xxi* which defines an external element. The compound input (up to six characters) is the name which will be printed in the results readout.

A combination printed in an existing list can be changed by the input of new data, or deleted by typing DL.

```
* ANM 1                                  Assemble names list from combination 1 (new list)

    ELM,COMPOUND
 1=      ,        :=  NA,NA2O
 2=      ,        :=  MG2,MGO
 3=      ,        :=  AL,AL2O3
 4=      ,        :=  SI,SIO2
 5=      ,        :=  S,SO3
 6=      ,        :=  K,K2O
 7=      ,        :=  CA2,CAO          Element/compounds listing
 8=      ,        :=  FE,FE2O3
 9=      ,        :=  C3,C3S
10=      ,        :=  C2,C2S
11=      ,        :=  CC,C3A
12=      ,        :=  CF,C4AF
13=      ,        :=  LS,LSF
14=      ,        :=  /                Terminate list assembly

*

* PNM                                    Print names list

      1       2       3       4       5       6       7       8       9       10

 0   NA      MG2     AL      SI      S       K       CA2     FE      C3      C2
       NA2O    MGO     AL2O3   SIO2    SO3     K2O     CAO     FE2O3   C3S     C2S

10   CC      CF      LS
       C3A     C4AF    LSF

*
```

Fig. 2.3F. Assembly of names list.

2.3.6. *Moduli list and sets*

For certain applications it is convenient for the output report to show moduli values in addition to, or in place of, element concentrations, where the moduli has a fixed relationship to a concentration.
Figure 2.3G shows the assembly of a moduli list and set.

The moduli set is assembled from the AMS i command, where i = 1 to 63, and is used to specify the name of the moduli, the number of decimals in the calculation, and the number of terms and the factors in the numerator and denominator.
A moduli set is used for the calculation of moduli from element channel measurement and concentration calculation output, in the form of:

$$\text{Moduli abc} = \frac{x_1C_1 \pm x_2C_2 \pm \text{etc.}}{x_3C_3 \pm x_4C_4 \pm \text{etc.}}$$

Moduli calculations can also be built up from partial (intermediate) moduli calculations, i.e. previously calculated moduli can be used as a term in the numerator or denominator. If in such case the printout of intermediate results is not required, select number of decimals = −1.

The names list defines the element and moduli names, but note that the element names for moduli calculation must be an external element, and be designated by an asterisk,e .g. LS*. The compound name can be up to six characters, and should not be the same as any channel names assembled by the ACH command.

The assembly of a moduli set is as follows:

NEW LIST	Is printed if the moduli set has not been assembled previously.
NAME =	The element name appearing in the ANM list must be given, and it should not be the same as any ACH channel names. This is an **external** element and is defined with an asterisk suffix.
NDEC =	−1 to 5. The number of decimals to appear in the calculation readout must be defined. If NDEC = −1 is selected, the modulus concerned will not be printed in the concentrations readout.
NR OF TERMS IN NUMERATOR =	0 to 31. The number of terms that will be used in the numerator of the moduli calculation must be defined.
NR OF TERMS IN DENOMINATOR =	0 to 31. The number of terms to be used in the denominator must be defined.
FACTOR CHANNEL	The factor is a number (x_1, x_2, etc.) to be input for use in the numerator part of the equation for N1, N2, etc., or a number (x_3, x_4, etc.) input for the denominator part for D1, D2, etc. For each factor the element channel (as MP list) must be given. The program will multiply each element countrate by its factor, and then calculate the moduli.

Refer to paragraph 2.8.1. for an example of an analysis involving moduli calculation.

```
* AML 10
NEW LIST
NR OF MODULI=   0 := 5
 1=    0 := 1
 2=    0 := 2
 3=    0 := 3
 4=    0 := 4
 5=    0 := 5
```

Assemble moduli list number 10

Moduli results in concentrations readout

Set numbers to be used for each moduli.

```
* AMS 5
NEW LIST
NAME=       := LS*
NDEC=   -1  := 1
NR OF TERMS IN NUMERATOR   =    0 := 1
NR OF TERMS IN DENOMINATOR=    0 := 3

       FACTOR   CHANNEL
N 1=   0.00000        :=100 CA2
D 1=   0.00000        :=2.8 SI
D 2=   0.00000        :=1.2 AL
D 3=   0.00000        :=.65 FE
```

Assemble moduli set number 5

Element name in names list (ANM)

One decimal in measurement readout

$$\text{Moduli (LS*)} = \frac{100 \times CA2}{2.8 \times SI + 1.2\ AL + 0.65\ FE}$$

```
* PMS 5
MSNR=  5      NAME= LS*    NDEC=  1

     NUMERATOR            DENOMINATOR
   FACTOR   CHANNEL     FACTOR   CHANNEL
100.00000    CA2       2.80000    SI
                       1.20000    AL
                       0.65000    FE
```

Print of moduli set

Fig. 2.3G. Assembly of a moduli list and moduli set.

2.3.7. *Limits list*

Using the limits list, and by selecting, option 9 (in the link program list ALP), a warning will be given if one or more of the sample measurement results is outside a specified limit. Those elements not defined in the limits list will not be checked.

An upper or lower percentage concentration value limit, or both, can be set, and if the value for the lower and/or upper limit is zero (0), a check of that limit is not made.

When the results are printed, an asterisk, will be printed against any element concentration which has been found to be outside a defined limit, an error message "RESULT(S) OUT OF RANGE", will be printed, and the terminal printer bell will ring.

The limits list is prepared from the command ALL i, where i = 1 to 63. The following input is required.

NRCH =	1 to 63. The number of channels to be subject to a limit check must be input.
CHAN =	Channel name, as in MP list.
LOW, LIMIT = UPP. LIMIT =	The limit value must be input, where 0 means no limit.

Note that if an upper limit only is required, the input should be xxi space 0 space U.L. value c.r.

```
* ALL 50                          Assemble limits list number 50
NEW LIST
NRCH=    0  :=1                   Only one channel to be checked

     CHAN  LOW.LIMIT  UPP.LIMIT
  1=            0.000      0.000  :=NI 8.01  Channel/limits input

* PLL 50                          Print limits list 50

LL 50     1 CHANNELS

CH        NI
LL        8.010
UL        0.000

*
```

Fig. 2.3H. Limits list assembly.

2.4. SAMPLE ANALYSIS

Before commencing analysis ensure that the parameter bank contents (CH sets, MP lists, etc.) are added to the identified databank on the "files" disc, see paragraph 2.1. – Databank/parameter bank handling.

Simplified measurement procedure

To measure unknown samples with a PW 1400 system, proceed as follows:

Check that the following parameters have been input:
- CH sets
- MP lists
- Job list, if required
- LP list (same number as MP list)
- RC sets - countrate correction
- CP list - for calculation of chemical concentrations
- NM list, ML list and MS sets, if required.

When the system is operational
- Select VACUUM, HELIUM or AIR atmopshere.
- Prepare samples and fit in sample holders.
- Type the commands PWR, SPN, CMD or BMD, RCM or RCJ or MPY, and PIN, as required.
- Load sample and give sample identification – this procedure will depend whether batch or continuous mode measurement is selected, and whether a sample changer is used. If I is not given (no identification) in the batch mode, use the SLP command to load the sampler before SMX.

A typical start measurement input, with results readout, is shown below:

```
* RES          Reset
                                  } Given as required
* BMD          Batch mode

* SMX 50                    Start measuring unknown sample with MP/LP 50
SAM.POS= 1 I                Sample to turret position 1 and identify
IDENT 1= STAINLESS 25       Sample identification

*
  MP 50  CP 50  STAINLESS STEELS                        22-03-1979 15.39
CONCENTRATIONS     STAINLESS 25

      SI          MN          S           P          NI          CR          MO
      0.60        1.88        0.018       0.027      11.99       17.41       2.42

      NB          TI
      0.01        0.02

*
```

Fig. 2.4A. Typical sample analysis

2.4.1. General

Measurements for quantitative analysis can be initiated from the terminal keyboard to the computer. The following routines can be used:

SMX	for the measurement of unknown samples, to obtain concentrations output.
SMM	to update the monitor results in buffer ratio measurements.
SPR	to obtain regression intensities of calibration standard samples, see paragraph 2.5.
SMA	to determine apparent concentrations on recalibration standard samples, see paragraph 2.6.

These measurements are initiated via the LP list(s), and use the measurement programs (MP lists) stored in the parameter bank, refer to paragraphs 1.3.2. and 1.4.3. for SMX and SMM.

PIN	to obtain a gross intensities output, in addition to concentrations.
NPI	to cancel PIN, i.e. no intensities output.
SJB	to commence measurement according to a job list, **with sample identification if I is input.**
WDD	enables subsequent measurement results to be stored on a disc in station 1. Also operative for SJB, in which case a job file is created.
STM or RTM	enable the transmission of results to a second output device.
FTM	resets STM and RTM.
SMR SSR SAR	initiates a recalibration routine, see paragraph 2.6.

Optional calculations and actions are described later:

PHD	in the asterisk mode a distribution plot is produced.
RCM RCJ MPY	recycle and averaging, refer to paragraph 1.4.6. and 1.4.8.
BMD CMD	batch/continuous mode operation, refer to paragraph 1.4.5.

2.4.2. Unknown samples

The measurement of unknown samples will commence when the SMX command is given, also see paragraph 1.4.1.

Measurement readout will show percentage concentrations for the elements when the countrate corrections and calculation parameters list is used. If the link program (LP) list has CPNR = 0 (no CP list), the readout will show intensities only in kilocounts per second (kcps).

A readout of intensities and concentrations is given if the PIN command is input before SMX, see figure 2.4B. This readout also shows the percentage counting statistical precision, i.e. $\epsilon = 100/\sqrt{\text{counts}}$ (for Mn $\epsilon = 100/\sqrt{31450} = 0{,}56$, Mn measured 10 seconds).

It is useful to compare the statistical error of unknown samples with those for monitor samples.

The optional calculations and actions, defined by the LP list, can include moduli calculation and readout of compound names.

If batch mode operation is chosen the free positions in the turret can be loaded with unknown samples, identified, and all samples are measured. If continuous mode operation is chosen one unknown sample is loaded to position 2 or 4, identified and analysis commences. During analysis another sample can be loaded, identified, the cap closes and the loading position plunger goes down to bring the sample through the airlock. After measurement the turret rotates to bring the sample to the loading position, and measurement starts on the next sample.

Start measuring unknown samples with MP/LP lists 50
Turret position 1 loaded, and identification to be given
Sample identification given.

```
* SMX 50
SAM.POS= 1 I
IDENT 1= STAINLESS 25

*
  MP 50  CP 50  STAINLESS STEELS                    22-03-1979 15.39
CONCENTRATIONS     STAINLESS 25

      SI          MN          S           P          NI          CR          MO
      0.60        1.88        0.018       0.027      11.99       17.41       2.42

      NB          TI
      0.01        0.02
```

Result shows element % concentrations.

Start measurement, as above.

```
* SMX 50
SAM.POS= 1 I
IDENT 1= STAINLESS 15

* PIN
```

Print gross intensities — **Note that the command can be given during measurement** but before readout.

```
*
  MP 50  CP 50  STAINLESS STEELS                    22-03-1979 15.46
GROSS INTENSITIES  STAINLESS 15

      MO          MO+         NB          NI          MN          CR          TI
     1327.        810.        848.      25878.      3145.       33026.      453.
      0.87%       2.48%       1.09%       0.14%       0.56%       0.12%      2.35%

      P2          P2+         S2-         S2          SI
       98.         32.         32.         72.       1052.
      1.60%       3.96%       3.93%       1.87%       0.69%

CONCENTRATIONS     STAINLESS 15

      SI          MN          S           P          NI          CR          MO
      0.54        1.76        0.015       0.032      9.00        18.59       0.07

      NB          TI
      0.00        0.00
```

Result shows gross intensities (countrate), with % counting statistical precision, and then concentration values.

Fig. 2.4B. Measurement of an unknown sample.

2.4.3. Monitor samples

The measurement of unknown samples in the buffer ratio mode (BRAT = YE) will be inhibited (and an error message given) unless the monitor sample is previously measured by the SMM command.
The monitor measurement results are then stored in a buffer for use in ratio calculation for unknown samples, and periodically the monitor sample is remeasured to update the stored intensities, see figure 2.4C. Whenever the stored intensities are updated the readout will show the percentage change in intensity value since the previous results.

A monitor buffer list must have been assembled (AMB command) before a monitor sample measurement command is given.

Direct ratio and buffer ratio measurements will correct for the effect of any drift of analysis results, if the monitor is a stable reference sample. The buffer results should be updated at regular intervals, but due to the high stability of the PW 1400 system these intervals can be comparatively long. It is generally preferred that a monitor sample be kept in the reserved position in the sample turret for buffer ratio measurements.

```
* LDM 1
```

first monitor measurement

```
* SMM 50

*
  MP 50  CP 50  NET INTENSITIES                          22-03-1979 12.46

      MO          NB          NI          MN          CR          TI          P2
    3005.       5218.      26837.       1037.      31122.      19306.         35.

      S2          SI
      33.       2266.
* SMM 50
```

monitor update measurement to also show the percentage change in intensity value.

```
*
  MP 50  CP 50  NET INTENSITIES                          22-03-1979 15.24

      MO          NB          NI          MN          CR          TI          P2
    3036.       5197.      26831.       1054.      31073.      19343.         36.
     1.02%      -0.40%      -0.03%       1.71%      -0.16%       0.19%       3.35%

      S2          SI
      32.       2267.
    -4.01%       0.06%

* ULM 1
```

Fig. 2.4C. Monitor sample measurements.

2.4.4. Moduli output

It is possible to arrange for the output report of unknown samples measurement to show the result of calculating a moduli. The calculation is described in paragraph 2.3.6., which shows the parameters to be input to the moduli list (ML) and moduli sets (MS). In addition to these lists, it is usually convenient to use compound names for some moduli in the output report. This requires the assembly of a names list as described in paragraph 2.3.5.

A moduli output will be printed when samples are measured via a link program (LP) list which calls for a moduli list (MODLST = 1 to 63). A typical example of list assembly and measurement result output for cement samples is given in paragraph 2.8.1. Moduli calculation can be used for other applications, such as: to print the carat value for gold in addition to % Au; to print grammes per litre NaCl in addition to % Na, etc.

An example of cement analysis results readout is shown in figure 2.4D, which includes compound names in the readout, e.g. FeO_3 instead of Fe.

```
* SMX 10                                  Start measurement (cement analysis)
SAM.POS= 1 I                              Sample in turret position 1
IDENT 1= C 2476/27                        Sample identification

* MP 10  CP 10  CEMENT ANALYSIS                        22-03-1979 09.55
CONCENTRATIONS      C 2476/27

      CAO        SIO2       AL2O3       FE2O3        SO3         MGO        NA2O
     64.3        21.4         5.5         3.3          2.1         1.7        0.65

      K2O         C3S         C2S         C3A         C4AF        LSF
     0.39        57.4        18.1         9.0         10.0        93.6
```

Fig. 2.4D. Example of moduli and compounds readout

2.4.5. Options

During the assembly of the link program (LP) list the request OPTION = appears, and one or more numbers can be typed in reply, as below:

OPTION = 0 No action, options set previously are inhibited.
= 1 Manual input of concentration(s) after the measurement.
= 2 Manual input of intensities after the measurement.
= 5 Normalisation to x %
= 6 Print the sum of the concentrations.
= 7 Element by difference.
= 8 Diluted samples
= 9 Concentration limits
= 10 Printout of element names.

In principle options can be combined by input of more than one option number, but note that some combinations do not make sense (e.g. 5 plus 7).

Option 1 - Manual input of concentrations

This option allows the manual (typed) input of the concentration value for an element which has not been measured and this value may be required for the matrix correction of other elements. The input value will usually have been determined by using another type of analysis, e.g. a wet chemical analysis.

As the element is not measured, a channel set is not required, but the LP listing must show this element as an "external element". This can have a normal element name symbol but must be denoted with an asterisk, e.g. C* for the element carbon having an externally determined concentration value — to be input for computer calculations. The value is input after the measurement of the intensities of the unknown sample(s), and before the calculation and output of concentration values. The computer request "GIVE CONCENTRATIONS OF SAMPLE (sample identification)" is typed with a listing of the external elements. The concentration value for each element (if known) is input, and the listing is repeated for any other samples which have been loaded and measured. The calculation and print of all element concentrations will include the manually input values. A maximum of 5 external elements for manual input of concentrations (or intensity) values is allowed.

Option 2 - Manual input of intensities

In a similar manner to option 1, the intensity value of elements can be typed in response to the request "GIVE INTENSITIES OF SAMPLE (sample identification)", input values in counts per second.

Option 1 can be combined with option 2, and when several external element values (maximum 5) are input the concentration listing of external elements will not include the elements which have previously had an intensity value manually input.

Options 3 and 4 are reserved and cannot be selected.

Option 5 - Normalisation to x %

After the measurement of a sample, and before readout, the concentrations are normalised, i.e. the concentrations are summed to give ΣC_i, and multiplied by a factor NF, where $NF = x/\Sigma C_i$. The sum of the normalised concentrations x has to be specified in the assembly of the LP list (SUM =), see figure 2.4E. If the sum is zero in the LP list, an input for the sum value will be requested after the measurement and before the results are printed.

The measurement readout will show the calculated NF factor ($= x/\Sigma C_i$), and a listing of **normalised** concentrations, see figure 2.4E.

```
* ALP 42
NRCH=    2 :=
OPTION=  0 := 5
SUM=    0.00 := 100
MBNR= 42 :=/
```

Assemble link program (for option 5)

$x = 100\ \% = NF \Sigma C_i$

Terminate LP list

```
* SMX 42
SAM.POS= 1 I
IDENT 1= BRASS 300A
```

Start measurement with MP/LP 42

Sample loaded, identified and measured after c.r.

Measurement results showing NF

```
*
  MP 42  CP 42  BRASS ANALYSIS                    28-03-1979 09.33
CONCENTRATIONS      BRASS 300A                NF 1.0008

      CU          ZN          SN          PB          FE          MN          AL
   58.87       40.10        0.25        0.26        0.10        0.15       0.085

      NI
    0.18
```

Normalised concentration values are printed ($\Sigma C_i = 100\%$)

Fig. 2.4E. Normalisation to x % (option 5).

Option 6 - Print the sum of the concentrations

The sum of the concentrations is calculated and printed in the analysis readout, see figure 2.4F.

```
* ALP 50
NRCH=    2 :=
OPTION=  0 := 6
MBNR= 50 :=/
```

Assemble LP list 50

Option 6 selected (ΣC_i)

```
* PLP 50
LPNR= 50      NRCH=  2      CPNR= 50      MODLST=  0      MBNR= 50
OPTION=  6

ELMNT P2    S2
RC     1     2
ABS    N     N
```

Print LP list

```
* SMX 50
SAM.POS= 1 I
IDENT 1= ST. STEEL #327
```

Start measurement

Results readout showing sum (ΣC_i) of concentrations.

```
*
  MP 50  CP 50  STAINLESS STEELS                  22-03-1979 18.20
CONCENTRATIONS      ST. STEEL #327            SUM 32.69

      SI          MN           S           P          NI          CR          MO
    0.60        1.58       0.019       0.029       11.45       18.35        0.04

      NB          TI
    0.64        0.00
```

Fig. 2.4F. Sum of the concentrations (option 6)

Option 7 - Element by difference

The concentration of **one** element which is **not included** in the measurement programs can be estimated by summing all the concentrations (ΣC_i) which have been measured, and subtracting this value from an input sum given in the LP list.

If the input sum is zero in the LP list, an input for this value will be requested after the measurement and before the results are printed.

```
* ALP 50                                    Assemble LP list
NRCH=   2 :=
OPTION=  0 := 7                            Option 7 selected
SUM=   0.00 := 100                         Sum = 100 % i.e. ΣCi + external element
ELMNT BY DIFF=        := FE*               Name of external element – with asterisk
NDEC=  0 := 2                              Number of decimal places in readout
MBNR= 50 := /

* PLP 50                                    Print LP list
LPNR= 50      NRCH=  2      CPNR= 50      MODLST=  0      MBNR= 50
OPTION=  7
SUM= 100.00  ELMNT BY DIFF= FE*           NDEC= 2

ELMNT P?    S2
RC      J    2
ABS     N    N

* SMX 50                                    Start measurement
SAM.POS= 1 1
IDENT 1= ST. STEEL #328

*                                          Results readout including Fe (external element)
  MP 50  CP 50  STAINLESS STEELS                          22-03-1979 18.28
CONCENTRATIONS     ST. STEEL #328

        SI          MN           S           P          NI          CR          MO
      0.84        1.61       0.016       0.018       20.07       25.10        0.07

        NB          TI          FE
      0.01        0.00       52.26
```

Fig. 2.4G. Element by difference (option 7).

Option 8 - Diluted samples

This option enables correction for sample dilution in the calculation of the concentrations.
After the measurement an input for the initial weight and the final weight of the sample is requested.
The calculated concentrations are multiplied by the dilution factor DF, where DF = final weight/initial weight, and this value is printed together with the corrected concentration values.

The use of this option with liquid samples is obvious but it can also be used for fused beads. In the example (figure 2.4H) the option is used to correct for a difference in sample to flux ratio of cement samples.
The calibration was performed on samples with weights 0,5 g sample + 2,5 g flux, and the unknown sample weights were 0,5 g + 2,7 g.

```
* ALP 10                                    Assemble link program
NRCH=    0 :=
OPTION=  0 := 8                             Option 8 selected
MBNR=    0 := /

* SMX 10                                    Start measurement
SAM.POS= 1 I
IDENT 1= C 2476/28

* INITIAL WEIGHT := 3.0                     Input of sample weights
FINAL   WEIGHT := 3.2

MP 10  CP 10  CEMENT ANALYSIS               Calculation results showing dilution factor and corrected
CONCENTRATIONS      C 2476/28               concentrations.
                                                    28-03-1979 13.55
                                            DF 1.07

      CAO        SIO2       AL2O3       FE2O3        SO3        MGO        NA2O
     63.0        23.0         3.7         4.9        2.0        1.6        0.25

      K2O         C3S         C2S         C3A       C4AF        LSF
     0.34        49.7        28.4         1.5       14.9       87.5
```

Fig. 2.4H. Diluted samples (option 8).

Option 9 - Concentration limits

Before the results are readout a check can be made whether the concentration of specified elements is outside defined limits. The element limits are defined in the LL list, see paragraph 2.3.7.
If a concentration is outside the limits range the value is identified with an asterisk in the readout, a message "RESULT(S) OUT OF RANGE" is printed, and the terminal bell is sounded - see figure 2.4J.

```
* ALL 50                                        Assemble limits list
NEW LIST
NRCH=    0 :=  1                               One channel for limit definition

     CHAN LOW.LIMIT UPP.LIMIT
   1=          0.000     0.000 :=  NI  8.01     Ni channel with lower limit = 8.01,
                                                upper limit not defined

* PLL 50                                        Print limits list

LL 50     1 CHANNELS

CH        NI
LL        8.010
UL        0.000

* ALP 50                                        Assemble link program
NRCH=    2 :=
OPTION=   0 :=  9                               Option 9 selected.
LLNR=    0 :=  50                               Limits list number to be input
MBNR=  50 :=  /

* SMX 50                                        Start measurement
SAM.POS= 1  I
IDENT 1= ST. STEEL #39

                                                Results readout (shows Ni out of limits range)
*
  MP 50  CP 50  STAINLESS STEELS                          28-03-1979  09.39
CONCENTRATIONS      ST. STEEL #39

        SI         MN          S          P         NI         CR         MO
      0.42       0.79      0.021      0.016      7.99*      16.32       0.02

        NB         TI
      0.02       0.01

*** RESULT(S) OUT OF RANGE                      Printed warning
```

Fig. 2.4J. Concentration limits (option 9).

Option 10 - Print of element names only

This option will prevent the printing of compound names in the results readout, i.e. only element names will be printed. The compound names assembled in the NM list will not be used, and the option eliminates the necessity to change the names list when only element names are to be printed.

2.4.6. Job program

A job program can be assembled in the same manner as described for the basic (microprocessor) spectrometer in paragraph 1.3.3. Note that parameter setting commands, such as SCH, COL, etc., can be input during the job assembly in J = dialog, even though these commands are not allowed during normal computer assembly when in the asterisk (*) mode.

Job measurement is also similar to the description in paragraphs 1.4.7. and 1.4.8., but note that sample identification can be given when computer control is used. When the start job SJB command is given the job list to be used must be defined as an argument. If an "I" argument is also input the operation is the same as for the SMX command, and a sample identification (up to 20 characters) will be requested.

2.4.7. Data to disc

Concentrations or intensities which are output from an SMX command sample measurement, can also be written to a flexible disc if the WDD command has been given previously. This command requires that a file name (identification) should be input, and the system will add a file extension identification, e.g. STEELS.C50.

Concentrations will be written to the disc when the CP list is used. In the link program list, if CPNR = 0 intensities will be recorded. Note that when CPNR = 0, the counting statistical error will be printed if the CST command is given for this disc file.

A typical readout for the write data to disc operation is shown in figure 2.4K.

```
* WDD DX1:STEELS                    Write data to disc in station 1, with identification STEELS.

* SMX 50                            Start measurement of unknown samples.
SAM.POS= 1 I
IDENT 1= STEEL #738

*
  MP 50  CP 50  STAINLESS STEELS                          28-MAR-79 16:28
CONCENTRATIONS     STEEL #738

      SI          MN           S           P          NI          CR          MO
      0.74        0.37      0.022       0.016      0.20        16.26       0.01

      NB          TI
      0.00        0.00

DATA TO FILE DX1:STEELS.C50        Output shows file name STEELS,
                                   file extension C50, and disc drive station number.
```

Fig. 2.4K. Write measurement data to disc.

Results from a job measurement can also be written to a disc from the WDD command. If the job list includes an SMX measurement, the output to disc is as described above. If the job list contains STS, CTS, SCT, SLF, SLS or SCH instructions the results are written to a file with the name identification as specified by WDD, and the file extension will be the job list number followed by a sequence number A to Z. A is given for the first time that data are written to the file by the SJB command, B for the second SJB data input, etc.
After 26 SJB inputs a different file name should be input.

A print job file (results) PJF command can be given when the file has been opened with OPF.

A typical job file readout is shown in figure 2.4L. The results were obtained from a job list measurement which comprised a step scan from 40^{o} to $46^{o}2\theta$, with a step size of $0{,}1^{o}$ and a 1 second measurement time per step.

```
* OPF DX1:SPECTR.54A
  128 RECORDS OF LENGTH:   6,  65 EMPTY RECORDS. FILE DATE:28-MAR-79
MODE= 8  JOBNR= 54     0 CYCLES

* PJF                          Print job file
JOB       JOBNR 54  CY   0  IDENT:                          28-MAR-79

  ANGLE     COUNTS      TIME       ANGLE     COUNTS      TIME
  40.000       457.    1.000       40.100       439.    1.000
  40.200       496.    1.000       40.300      1292.    1.000
  40.400      2564.    1.000       40.500      2312.    1.000
  40.600      1117.    1.000       40.700       657.    1.000
  40.800       513.    1.000       40.900       447.    1.000
  41.000       416.    1.000       41.100       440.    1.000
  41.200       527.    1.000       41.300       512.    1.000
  41.400       831.    1.000       41.500      1941.    1.000
  41.600      7186.    1.000       41.700     17420.    1.000
  41.800     20286.    1.000       41.900     12733.    1.000
  42.000      4844.    1.000       42.100      1492.    1.000
  42.200       675.    1.000       42.300       489.    1.000
  42.400       395.    1.000       42.500       406.    1.000
  42.600       416.    1.000       42.700       529.    1.000
  42.800       971.    1.000       42.900      2255.    1.000
  43.000      3211.    1.000       43.100      2222.    1.000
  43.200      1114.    1.000       43.300       853.    1.000
  43.400       773.    1.000       43.500       754.    1.000
  43.600      1390.    1.000       43.700      2375.    1.000
  43.800      2143.    1.000       43.900      1089.    1.000
  44.000       554.    1.000       44.100       384.    1.000
  44.200       337.    1.000       44.300       338.    1.000
  44.400       337.    1.000       44.500       398.    1.000
  44.600       514.    1.000       44.700       996.    1.000
  44.800      3233.    1.000       44.900      9532.    1.000
  45.000     14184.    1.000       45.100     10908.    1.000
  45.200      4994.    1.000       45.300      1665.    1.000
  45.400       672.    1.000       45.500       460.    1.000
  45.600       399.    1.000       45.700       446.    1.000
  45.800       627.    1.000       45.900       851.    1.000
  46.000       749.    1.000

*
```

Fig. 2.4L. Job file readout.

```
* PLS          Plot a spectrum (no argument = all scans in the file).
PLOTMODE:
1 = JOBFILE, ANGLE PRINTED ; 2 = JOBFILE, KCOUNTS PRINTED
PLOTMODE = 1   := Select either angle or counts as X-axis
LAY-OUT OF PLOT:
POINTS = 1; HISTOGRAM = 2
LAYOUT = 1   := Select either point plot or a histogram
ELEMENT
Y-SCALE-RANGES: .1/.2/.5/1/2/5/10/20/50/100/200/500/1000
Y-SCALE=       50.0:=20   Computer suggests full scale = 50 kcps, but 20 chosen for improved resolution
          ! FS =    20.000----------------------------------------------------------------------
   40.100 !*
   40.200 !*
   40.300 !   *
   40.400 !       *
   40.500 !      *
   40.600 !  *
   40.700 ! *
   40.800 !*
   40.900 !*
   41.000 !*
   41.100 !*
   41.200 !*
   41.300 !*
   41.400 ! *
   41.500 !     *
   41.600 !                        *
   41.700 !                                                    *
   41.800 !                                                          *
   41.900 !                                          *
   42.000 !                  *
   42.100 !    *
   42.200 ! *
   42.300 !*
   42.400 !*
   42.500 !*
   42.600 !*
   42.700 !*
   42.800 !  *
   42.900 !       *
   43.000 !          *
   43.100 !       *
   43.200 !  *
   43.300 ! *
   43.400 ! *
   43.500 ! *
   43.600 !   *
   43.700 !        *
   43.800 !       *
   43.900 !  *
   44.000 !*
   44.100 !*
   44.200 !*
   44.300 !*
   44.400 !*
   44.500 !*
   44.600 !*
   44.700 !  *
   44.800 !           *
   44.900 !                              *
   45.000 !                                          *
   45.100 !                                    *
   45.200 !                  *
   45.300 !    *
   45.400 ! *
   45.500 !*
   45.600 !*
   45.700 !*
   45.800 ! *
   45.900 ! *
SAME PLOT?= NO :=
NEXT PLOT?= YE :=N
```

* *Figure 2.4 M Plot of a step scan spectrum*

2.4.8. Statistics operation

Sample analysis results can be evaluated by using a calculate statistics command CST. This routine is a very useful extension of the normal analysis procedure, where it can show analysis results on a day, week, etc. basis.

The measurement results must be in a concentrations file in the "file" disc placed in station 1. First open the file by giving the OFF command with the file identification and file extension, see figure 2.4M.

When the CST command is given the readout will show columns for each element, as follows:

MAXIMUM	— maximum value (%C or kcps), and the sample number between brackets.
MINIMUM	— minimum value (and sample number)
AVERAGE	— the calculated average value
SIGMA	— the standard deviation around the average value
COV	— the coefficient of variance

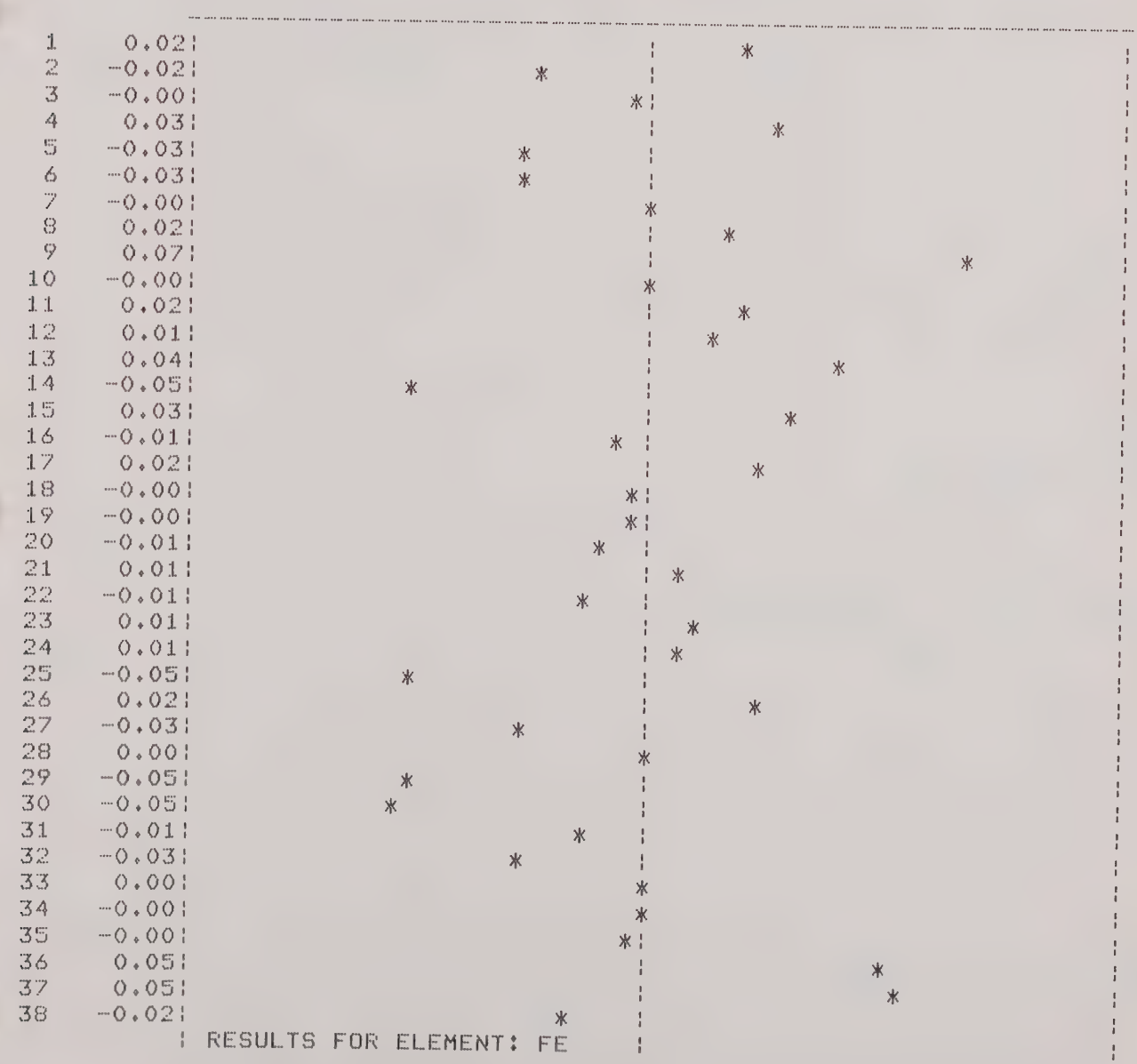
If CP = 0 in the LP list assembly (see OPF readout), there will only be intensity data in the file (in kcps), and the CST readout will additionally show the calculation of the counting statistical precision (1 sigma level) as C.ST.ERR.

If a plot of results is required type Y or YE for PLOT = NO =, and the sample number and deviation from the average value (shown dotted) will be plotted, for a specified element, see figure 2.4N.

```
* OPF DX1:STATIS.CO3                    Open file in disc station 1 with identification and extension
   90 RECORDS OF LENGTH:  17,  51 EMPTY RECORDS. FILE DATE:28-MAR-79
MODE= 1  MP=  3  CP=  0    38 SAMPLES      Note CP = 0, results in kcps
  3 CHANNELS: NI    FE    CR
           400.0 100.0 400.0               Measurement times

* CST                                     Calculate statistics
ELM      MAXIMUM          MINIMUM          AVERAGE     SIGMA      COV      C.ST.ERR

NI      37.083 ( 14)     37.048 (  2)     37.065     0.0085    0.023%     0.026
FE     249.555 (  9)    249.252 ( 30)    249.387     0.0718    0.029%     0.020
CR      30.128 ( 13)     30.083 ( 24)     30.111     0.0104    0.035%     0.029
PLOT=NO:=

*
```

Fig. 2.4M. Calculate statistics.

```
* OPF IX1:STATIS.CO3                          Open file
   90 RECORDS OF LENGTH:  17,  51 EMPTY RECORDS. FILE DATE:28-MAR-79
MODE= 1  MF=  3  CP=  0    38 SAMPLES
  3 CHANNELS: NI     FE     CR
            400.0  100.0  400.0


* CST                                         Calculate statistics
ELM      MAXIMUM           MINIMUM          AVERAGE     SIGMA      COV      C.ST.ERR

NI      37.083 ( 14)     37.048 (  2)      37.065     0.0085    0.023%      0.026
FE     249.555 (  9)    249.252 ( 30)     249.387     0.0718    0.029%      0.020
CR      30.128 ( 13)     30.083 ( 24)      30.111     0.0104    0.035%      0.029
PLOT=NO:=Y                                  Plot results
PLOT ALL ELEMENTS=NO:=                      For defined element(s)
ELEMENT := FE                               Results for Fe chosen
```




```
ELEMENT := /
```

2.4.9. Transmission to a second output device

A second and third peripheral can be connected to the computer in addition to the main terminal, to receive output data only. Thus it is possible to transmit analysis results to a second terminal (possibly in a different location) and the operator at the main terminal can approve or inhibit the transmission to the second device.

Referring to paragraph 2.1.2., the assemble system parameters (ASP) command and input must be given before the system is used. This defines the parameters of the main terminal and the second and third (output only) devices.

Because the microprocessor software operation is independent of the computer software, it is possible to connect an output device to the microprocessor second interface (optional) and the description in paragraph 1.5. will apply, but note that only microprocessor results will be output i.e. counts and time data only.

When a second or third output device is connected **to the computer,** and is specified by the ASP command, the following commands can be used, see figures 2.4P and Q.

STM	Transmit results to a second output device. Active until reset by FTM.
RTM	Request whether transmission of analysis results to a second output device is required. After analysis and readout at the main terminal the operator can decide whether the results should be output to the second device. Active until reset by FTM.
FTM	Reset of STM or RTM command.

```
* PSP                                          Print of system parameter
TERMINALTYPE  TT

CONCENTRATION AND LISTING OUTPUT DEVICES :
 1 = TT   WIDTH =  80
 2 = LP   WIDTH = 132          Line printer as second device

* RTM                         Request transmission to second output device

* SMX 50                      Start measurement
SAM.POS= 1 I
IDENT 1= STEEL #739


*
  MP 50  CP 50  STAINLESS STEELS                          28-MAR-79 16:50
CONCENTRATIONS      STEEL #739

      SIO2          MN             S             P          NI          CR          MO
      0.86          1.61       0.023         0.018       20.10       25.11       0.07

      NB            TI
      0.00          0.00

START TRANSMISSION = YE :=    Results accepted for transmission to second device
```

Fig. 2.4P. Output at main terminal.

```
MP 50  CP 50  STAINLESS STEELS                          28-MAR-79 16:50
CONCENTRATIONS      STEEL #739

      SIO2          MN             S             P          NI          CR          MO          NB          TI
      0.86          1.61       0.023         0.018       20.10       25.11       0.07        0.00        0.00

*
```

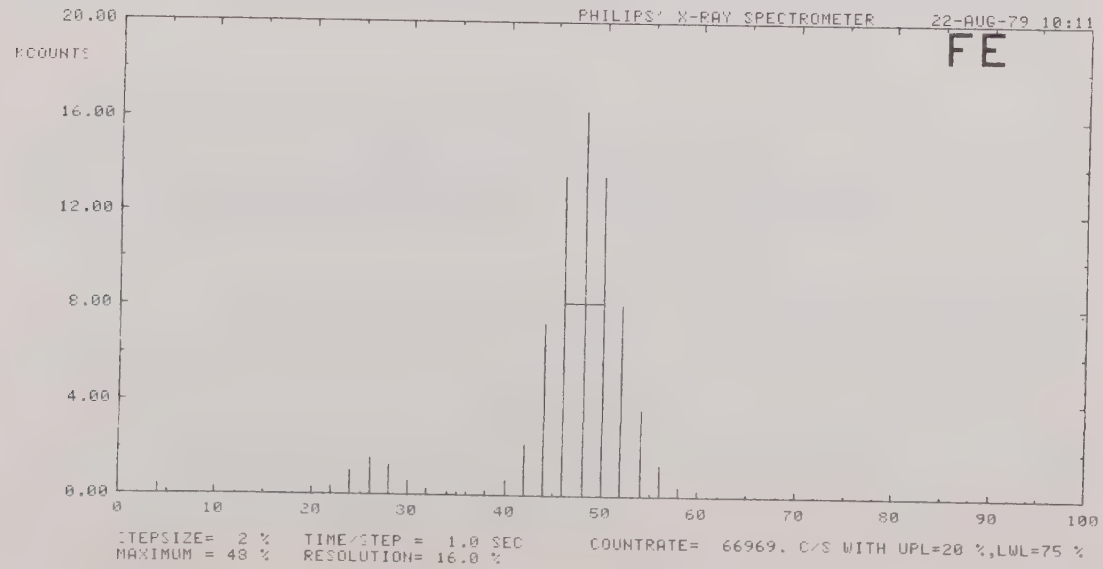
2.4.10. Pulse height distribution

A pulse height-distribution is obtained by plotting the intensity in a narrow window when a channel lower level is varied from 0 to 100 %. This procedure is fully described in paragraph 1.4.11., and figure 1.4S shows a typical chart recording, and figure 1.4R shows a microprocessor PHD readout.

When the computer is connected the PHD output is similar to figure 2.4R if the output is to a printer. If the output is to a graphical terminal the readout is similar to figure 2.4S.

```
* PHD CU
WINDOW : 5 :=>
TIME : 1.0 :=>

*
 0---
 2-----------------------------------------------------------------------|-----------------------------------------------------------------------
 4-----------------------------------------------------------------------|-----------------------------------------------------------------------
 6--
 8--
10
32
34
36
38
40
42
44
46
48-----------------------------------------------------------------------|-----
50-----------------------------------------------------------------------|-----------------------------------------------------------------------
52-----------------------------------------------------------------------|-----------------------------------------------------------------------
54-----------------------------------------------------------------------|-----------------------------------------------------------------------
56-----------------------------------------------------------------------|-----------------------------------------------------------------------
58
60
62
64
66
94
96
98
CU     WINDOW=   2%   MAXIMUM= 53%    RESOLUTION= 18.1   20-03-1979 12:58:50
INTERNAL SETTING INTENSITY=   84814. COUNTS/SEC
```

Fig. 2.4R. PHD output to a printer (from computer).



2.5. SYSTEM CALIBRATION

The calculation of chemical concentrations, from the measured element intensities of an unknown sample, is only possible if a calculation parameters (CP) list is used. The CP list will require an input of D and E constants, and can have sets of matrix correction constants. The D and E constants are **instrument** dependent, and after the initial calibration routine, can be periodically updated by a recalibration routine as described in paragraph 2.6. The matrix correction constants are **sample type** dependent, and the alpha constants (see paragraph 2.1.3.) are fixed and known for any sample and spectrometer combination. Tables showing alpha values for the "De Jongh" formula can be obtained from Philips or they can be calculated by a regression analysis procedure, which is described below. If the Rasberry-Heinrich and Lucas-Tooth Pyne calculation models are used for sample analysis the beta values can only be obtained from the regression analysis routine.

Regression is the procedure for setting the calibration line, see fig. 2.1G. It requires the measurement of calibration (standard) samples which are similar to the range of unknown samples to be analysed. Accurate concentrations data for the calibration samples must be available.

The measurement of the calibration standards commences from the **SPR** command (start prepare regression) according to an MP/LP measurement program, and the resultant intensities are written to a flexible disc.

When all the standards have been measured, the known chemical concentrations data are manually input to the disc file (containing the intensities), from the command **ACD** (assemble concentrations data).

Now the sets of intensity and concentrations data are read into the memory by the command **SRI** (start regression /input). At this stage the regression calculation model is chosen (DJ, LP or RH).
The regression calulation is initialed by **SRA** (start regression), which will output the regression constants (E= slope and D = intercept of the calibration line). The output also shows values for SIGMA and K which indicate the goodness of the fit of the calibration line.

The standard deviation - σ is given by:

$$\text{SIGMA } (\sigma) = \sqrt{\frac{\Sigma_i^n \ (C_{chem.} - C_{calc.})^2}{n-k}} \quad \text{weight \%}$$

where n = the number of samples.
k = the number of regression coefficients. For a straight line k = 2, also if all the influence coefficients (alphas) have been determined independently, In general, k = 2 plus the number of influence coefficients found by regression analysis.

Analytical deviations will generally depend on the level of concentration, and will be greater (in weight %) for the higher concentrations. Thus, sigma $\approx K\sqrt{C}$, where K is a proportionality factor.

The regression program is arranged to reduce the K factor to a minimum, rather than sigma, which is useful when analysing large ranges of element concentrations. This implies a weighting of errors. Refer to the Application Report "X-ray spectrometry in the metals industry".

Interelement correction factors can be calculated using the commands **CAL** and **CBT** (calculate alpha/beta), or known correction factors can be entered using **FAL** and **FBT** (fix alpha/beta). Sample intensity/concentration data can be deleted from the calculation by **DSA**, or reinserted by **ISA** (delete/insert sample). Intensity and concentration data can be corrected if an error has occured during input using **CID** and **CCD** (correct intensity/ concentration data). Also the equivalent background can be adjusted by **CEB** (change equivalent background).

A detailed readout of the regression results is given from **PRL** (print results list). This listing shows columns for each sample (numbered from 1 upward), as follows:

INTENSITY	As input to the file from the standard sample measurement (SPR command)
CHEMICAL CONCENTRATION	As manually input (ACD command)
CALCULATED CONCENTRATION	based on the intensity values and using the available D, E, α and β values, in the selected calculation model.

CONCENTRATION DIFFERENCE	The difference between the chemical and calculated values.
CHEMICAL APPARENT CONCENTRATION	Equal to $C / (1 + \Sigma \alpha C)$, from the correction formula $C = (D + ER)(1 + \Sigma \alpha C)$.
CALCULATED APPARENT CONCENTRATION	Equal to $C_A = (D + ER)$.
IDENTIFICATION	Identification of the standard samples, as input by the SPR command.

When the regression results are satisfactory they can be automatically transferred to the CP list by giving **SRR** (save regression results). The regression routine then continues for the next element by giving **NRE** next regression element.

If a graphical terminal is connected the regression results can be plotted with **PLT**, which aids evaluation of the results.

2.5.1. Prepare for regression analysis

The regression analysis calculation routine requires intensity and concentration values for each element in the set of standard samples. These data are stored in a file on the files disc in disc drive 1.

When the calibration standard samples are ready for analysis, the system disc must be in station 0, and the files disc in disc drive 1. Give a write data to disc command WDDxxxxxx, where xxxxxx is a six character identification relating to the type of samples to be analysed, e.g. STEELS as the example in figure 2.5A.

Now give the SPR (start prepare regression) command, and define the measurement/link program to be used. This number will be incorporated in the file type identification.

The dialog requests the turret positions and sample identification to be defined, and the standard samples are loaded and measured. The readout-shows the intensity values which have been written to the files disc. Repeat the procedure (SPR) until all samples have been measured, then give NDD (no data to disc).

The regression intensities file on the files disc must now be opened by giving the OPF xxxxxx command, where xxxxxx is the same identification as given with WDD above.

Now give the ACD (add concentration data) command to add the known chemical concentration values of the standard samples to the file xxxxxx in the files disc, see figure 2.5B. The dialog will request an input of concentration values for **all** elements in all the standard samples which have been measured, so type the known value or give a carriage return (or zero).

Note that most of the following readouts were prepared from the P851 computer software, using a file identification STL, and for the X14-D (PDP11) software the file identification, date and time have a slightly different format, as figure 2.5A.

```
* WDD DX1:STEELS
```

Write data to disc in station 1, with identification STEELS

```
* SPR 50
SAM.POS= 1 2 3 4 1
IDENT 1= SS-61
IDENT 2= SS-62
IDENT 3= SS-63
IDENT 4= SS-64

*
  MP 50  CP 50
   CYCLE   1  22-MAR-79 13:08
INTENSITIES         SS-61

      MO          NB          NI          MN          CR          TI          P2
   0.03421     0.15770     0.66691     1.43867     0.92323     0.01819     0.69968

      S2         SIO2
   1.27439     0.36980

DATA TO FILE DX1:STEELS.R50

INTENSITIES         SS-62

      MO          NB          NI          MN          CR          TI          P2
   0.05041     0.19547     1.33249     1.42797     0.76928     0.01659     0.49855

      S2         SIO2
   1.68475     0.36934

DATA TO FILE DX1:STEELS.R50

INTENSITIES         SS-63

      MO          NB          NI          MN          CR          TI          P2
   0.03860     0.17244     1.01987     1.48324     1.06837     0.01714     0.68910

      S2         SIO2
   1.87100     0.38851
```

Start prepare regression

Sample loading and identification

Note file extension

Routine continues for all samples

Fig. 2.5A Prepare for regression — intensities input.

```
* OPF DX1:STEELS.R50
   16 RECORDS OF LENGTH: 47,   7 EMPTY RECORDS. FILE DATE:22-MAR-79
MODE= 3  MF= 50  CF= 50     8 SAMPLES
  9 CHANNELS: MO    NB    NI    MN    CR    TI    P2    S2    SI
```

Open file STEELS.R50 on disc in station 1.

```
* ACD
```

Assemble concentrations data

```
SAMPLE  1  SS-61
MO    := .018
NB    := .000
NI    := 6.26
MN    := .78
CR    := 15.2
TI    := .000
P2    := .016
S2    := .016
SI    := .42

SAMPLE  2  SS-62
MO    := .02
NB    := .028
NI    := 12.45
MN    := .8
CR    := 12.8
TI    := .000
P2    := .015
S2    := .02
SI    := .44

SAMPLE  3  SS-63
MO    := .017
NB    := .005
NI    := 9.49
MN    := .79
CR    := 18.7
TI    :=
P2    := .016
S2    := .02
SI    := .45

SAMPLE  4  SS-64
MO    := .014
NB    :=
NI    := 20.7
MN    :=
CR
```

Continued for all samples.

Concentrations input (if available)

```
SS-66
      .43
      .006
   := 9.48
   := .81
   := 17.6
I  := .002
P2 := .02
S2 := .023
SI := .51

SAMPLE  7  SS-67
MO    := .041
NB    := 1.02
NI    := 9.52
MN    := .87
CR    := 17.8
TI    :=
P2    := .016
S2    := .018
SI    := .5

SAMPLE  8  SS-68
MO    := .033
NB    :=
NI    := 9.33
MN    := 1.59
CR    := 18.55
TI    :=
P2    := .027
S2    := .028
SI    := 1.42
```

Fig. 2.5B. Add concentrations data to file.

2.5.2. Regression analysis procedure

The intensity and concentration values for the standard samples must be input to the computer for the regression analysis routine to calculate D and E constants and matrix correction factors, see figure 2.5C. Regression analysis is normally carried out on a regression file after the OPF command. Off-line regression analysis is possible if no file is opened using OPF before giving the command SRI.

Give the command SRI (start regression input). The dialog first requests the input (DJ, LP or RH) to define the calculation model to be used, refer to paragraph 2.1.3.

The LOAD ALL ELEMENTS request follows, and requires an answer YE (c.r. = yes), or NO if only specified elements are to be included in the routine.

After printing the list of elements that are now loaded into the computer the request REGR. ELMNT = requires an input of the first element for regression analysis. Note that the sequence of element concentrations printed after sample analysis is determined by the order of elements input to the CP list. This order is normally determined by the command SRR (save regression results) given after a regression analysis produces satisfactory results. Thus, the order of elements for the REGR. ELMNT input will determine the order of concentration result output.

```
* SRI                                        Start regression input
MODEL= DJ :=                                 Select mathematical model
LOAD ALL ELEMENTS =YE:=                      Decide if all elements (on disc in station 1) to be used in regression
LOADED ELEMENTS:    MO     NB     NI     MN     CR     TI     P2     S2     SI

  8 OF THE   8 SAMPLES LOADED
REGR. ELMNT := SI                            Select first element for regression analysis

* SRA                                        Regression analysis started
ELEMENT= SI        MODEL= DJ     SIGMA=    0.01039     K=    0.01358
                                             Regression results for silicon
       D              E
    -0.04110       1.25447

FILE:STLR50,1 (22-03-1979)   }               See note on page 2.55 D
DATE:22-03-1979 13.48        }
```

Fig. 2.5C. Start regression input.

The command SRA (start regression analysis) starts the mathematical process of calculating the best fit for an element calibration line through the intensity/concentration points for the standard samples. The calculation takes into account any interelement correction factors which have been input.

The printout shows values for the D and E regression constants, and the goodness of fit expressed as SIGMA and K values, see figure 2.5D.

The command PRL prints a detailed list for the individual samples with respect to the calibration line. The calculated apparent concentrations can be used in the recalibration routine (paragraph 2.6.), therefore, it is advisable to retain the PRL printout from the final regression (just before SRR).

If interelement corrections are applied the factors will be printed in the SRA output, see figure 2.5E. If known factors have been input these will be marked with an asterisk (from FAL and FBT). If these factors are calculated in the regression (CAL and CBT) an asterisk will not be printed.

If the calibration point for a standard sample is not acceptable, that sample can be deleted from the calculation and SRA repeated to determine whether the analysis results are improved. The PRL readout will show an asterisk against those samples which have not been included in the calculation.

```
* SRA                                                    Start regression analysis
ELEMENT= SI       MODEL= DJ     SIGMA=    0.01039     K=    0.01358

      D             E
   -0.04110       1.25447

FILE:STLR50,1 (22-03-1979)
DATE:22-03-1979 13.48

* PRL                                                    Print results list
NR INTENSITY --------CONCENTRATION---------  APPARENT CONCENTR. IDENTIFICATION
             CHEMICAL CALCULATED    DIFF.    CHEMICAL CALCULATED
 1   0.370   0.42000   0.42281   0.00281     0.42000   0.42281 SS-61
 2   0.369   0.44000   0.42223  -0.01777     0.44000   0.42223 SS-62
 3   0.389   0.45000   0.44628  -0.00372     0.45000   0.44628 SS-63
 4   0.391   0.45000   0.44944  -0.00056     0.45000   0.44944 SS-64
 5   0.567   0.67000   0.67015   0.00015     0.67000   0.67015 SS-65
 6   0.450   0.51000   0.52340   0.01340     0.51000   0.52340 SS-66
 7   0.439   0.50000   0.51003   0.01003     0.50000   0.51003 SS-67
 8   1.160   1.42000   1.41456  -0.00544     1.42000   1.41456 SS-68
```

Fig. 2.5D. Regression analysis for Si without interelement correction.

```
* SRA                                                    Start regression analysis
ELEMENT= CR       MODEL= DJ     SIGMA=    0.11104     K=    0.02510

      D             E       ALPHA(MO )  ALPHA(NB )  ALPHA(NI )  ALPHA(MN )
   0.31563      12.48714      4.22700*    3.93200*    0.77000*    0.59000*

 ALPHA(CR )  ALPHA(TI )  ALPHA(P2 )  ALPHA(S2 )  ALPHA(SI )
   1.49500*    5.92900*    1.61300*    2.23000*    1.22600*

FILE:STLR50,1 (22-03-1979)
DATE:22-03-1979 15.06

* PRL                                                    Print results list
NR INTENSITY --------CONCENTRATION---------  APPARENT CONCENTR. IDENTIFICATION
             CHEMICAL CALCULATED    DIFF.    CHEMICAL CALCULATED
 1   0.923  15.20000  15.23826   0.03826    11.81437  11.84410 SS-61
 2   0.769  12.80000  12.89799   0.09799     9.84635   9.92173 SS-62
 3   1.068  18.70000  18.63349  -0.06651    13.70531  13.65656 SS-63
 4   1.304  25.60000  25.77364   0.17364    16.48265  16.59445 SS-64
 5   1.033  18.45000  18.39801  -0.05199    13.25308  13.21573 SS-65
 6   0.943  17.60000  17.54050  -0.05950    12.12912  12.08811 SS-66
 7   0.999  17.80000  17.81247   0.01247    12.77656  12.78551 SS-67
 8   1.044  18.55000  18.40187  -0.14813    13.45755  13.35008 SS-68
```

Fig. 2.5E. Regression analysis for Cr with interelement correction.

If a HP 2648A graphics terminal is connected, plots can be produced after SRA to study the regression results, using the command PLT. (Hewlett Packard HP 2648A or HP 2649C).
Input to specify the X-axis and Y-axis is then requested (see fig. 2.5F), and after the input this plot appears on the screen, see fig. 2.5H and J.

```
* PLT                                          Plot parameters
SELECT Y-AXIS:
1=CHEMC(CR  ); 2=CHEM-APPC(CR  ); 3=CALCC(CR  ); 4=CHEMC/R(CR  );
5=DIFF C(CR  ); 6=DIFF C/R(CR  )
Y-AXIS :=2                                     Y-axis = chemical apparent concentrations
SELECT X-AXIS:
1=CHEMC(CR  ); 2=R(CR  ); 3=CHEMC(XX)
X-AXIS :=1                                     X-axis = chemical concentrations
```

Fig. 2.5F. Plot parameters input.

If X-axis 2 is selected and Y-axis 1, 2 or 3, the regression line can also be added to the plot by typing:
L carriage return. A grid can be added to the screen by typing G carriage return.
The screen is cleared with c.r. and the next plot can be made by repeating PLT.

Note that a plot can only be produced with a graphics terminal (not VDU) and GT must be specified in ASP, see fig. 2.5G.

```
* PSP                                          Print system parameters
TERMINAL TYPE= GT                              Graphical terminal specified
LINES/SCREEN = 24


CONCENTRATION AND LISTING OUTPUT DEVICES :
 1 = TT  WIDTH =  80
 2 = LP  WIDTH = 132
```

Fig. 2.5G. System parameters for graphical terminal.

```
* SRA                                    Start regression analysis
ELEMENT= CR       MODEL= DJ     SIGMA=   0.11104     K=   0.02510

      D             E        ALPHA(MO )  ALPHA(NB )  ALPHA(NI )  ALPHA(MN )
   0.31563      12.48714      4.22700*    3.93200*    0.77000*    0.59000*

 ALPHA(CR )  ALPHA(TI )  ALPHA(P2 )  ALPHA(S2 )  ALPHA(SI )
   1.49500*    5.92900*    1.61300*    2.23000*    1.22600*

FILE:STLR50,1(22-03-1979)
DATE:22-03-1979 16.06

* PRL                                    Print results list
NR INTENSITY --------CONCENTRATION---------  APPARENT CONCENTR. IDENTIFICATION
             CHEMICAL CALCULATED    DIFF.   CHEMICAL CALCULATED
 1   0.923  15.20000  15.23826  0.03826   11.81437  11.84410 SS-61
 2   0.769  12.80000  12.89799  0.09799    9.84635   9.92173 SS-62
 3   1.068  18.70000  18.63349 -0.06651   13.70531  13.65656 SS-63
 4   1.304  25.60000  25.77364  0.17364   16.48265  16.59445 SS-64
 5   1.033  18.45000  18.39801 -0.05199   13.25308  13.21573 SS-65
 6   0.943  17.60000  17.54050 -0.05950   12.12912  12.08811 SS-66
 7   0.999  17.80000  17.81247  0.01247   12.77656  12.78551 SS-67
 8   1.044  18.55000  18.40187 -0.14813   13.45755  13.35008 SS-68

* PLT                                    Plot results
SELECT Y-AXIS:
1=CHEMC(CR  ); 2=CHEM-APPC(CR  ); 3=CALCC(CR  ); 4=CHEMC/R(CR  );
5=DIFF C(CR  ); 6=DIFF C/R(CR  )
Y-AXIS := 2
SELECT X-AXIS:
1=CHEMC(CR  ); 2=R(CR  ); 3=CHEMC(XX)
X-AXIS := 1
```

Plotter output

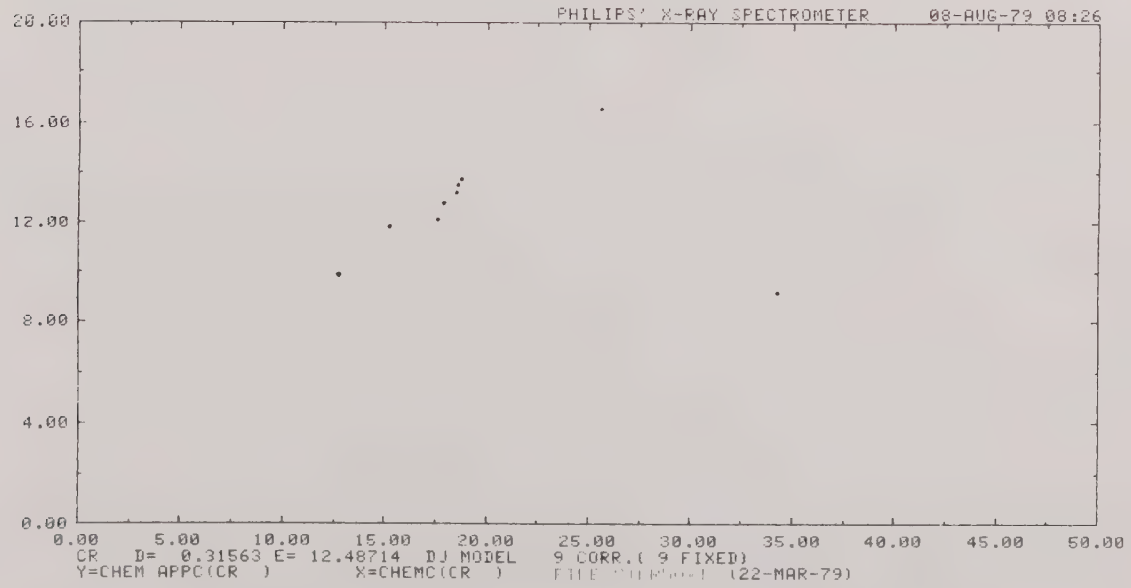
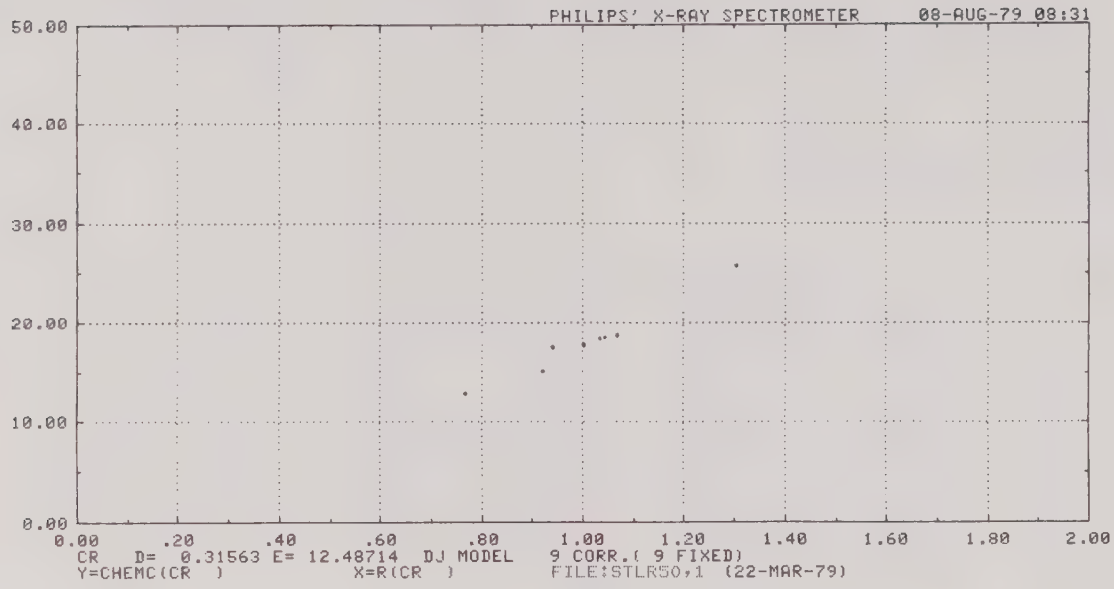


Figure 2.5H. Regression analysis and plot of results (chemical apparent concentrations versus chemical concentrations).

Chemical concentrations versus intensities



Difference (calculated-chemical) concentration of Cr/intensity Cr versus chemical concentration of interfering element XX (Ni).

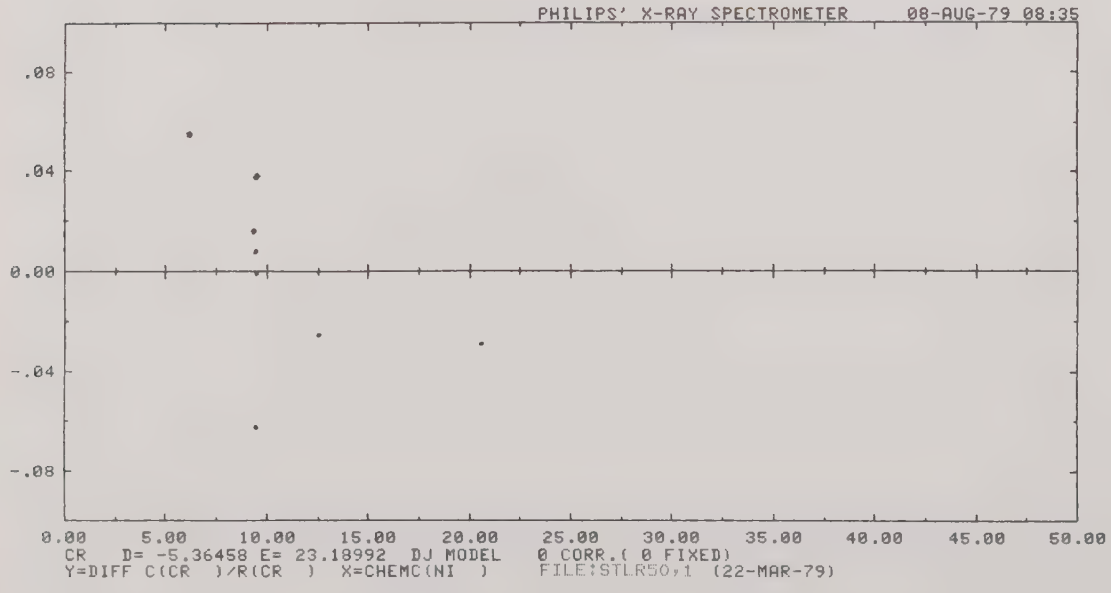


Fig. 2.5J Different plot outputs

The commands CAL, CBT, FAL, FBT, RCF are given before a start regression analysis, see figures 2.5K and 2.5L.

CAL, and CBT, if the RH model is selected, will calculate an interelement factor (s) in addition to the regression constants D and E. Known correction factors can be entered using FAL, and FBT for the RH model. Philips can supply correction factors for the DJ model, which have been mathematically derived from physical data.

If the mathematical calculation of an interelement correction factor does not succeed, i.e. the iterative process does not lead to convergence, a warning will be printed, figure 2.5K.

Previously set correction factors, either CAL, CBT, FAL or FBT, can be reset by RCF.

```
* SRA                                              Start regression analysis
ELEMENT= CR       MODEL= DJ     SIGMA=   0.72824     K=    0.17171

      D              E                             Unsatisfactory results
   -5.36458      23.18992

FILE:STLR50,1(22-03-1979)
DATE:22-03-1979 15.03

* CAL NI                                           Try to improve by calculating the alpha for Ni


* SRA
ELEMENT= CR       MODEL= DJ     SIGMA=   0.60886     K=    0.14652

      D              E        ALPHA(NI )           Still unsatisfactory
   -3.28391      19.93202      0.64369

FILE:STLR50,1(22-03-1979)
DATE:22-03-1979 15.04

* RCF                                              Reset CAL NI


* CAL CR                                           Calculate alpha for CR


*SRA                                               Start regression analysis
***NO CONVERGENCE                                  but routine cannot solve equations
FILE:STLR50,1(22-03-1979)                          to produce correction constants.
DATE:22-03-1979 15.04
```

Fig. 2.5K. Alpha calculation, reset, and no convergence in calculation.

```
* FAL SI 1.226

* FAL P2 1.613

* FAL S2 2.23

* FAL TI 5.929

* FAL CR 1.495

* FAL MN .59

* FAL NI .77

* FAL NB 3.932

* FAL MO 4.227
```

Input of physical or theoretical alphas

```
* SRA
ELEMENT= CR       MODEL= D_     SIGMA=    0.11104     K=    0.02510

      D             E       ALPHA(MO )  ALPHA(NB )  ALPHA(NI )  ALPHA(MN )
    0.31563     12.48714     4.22700*    3.93200*    0.77000*    0.59000*

 ALPHA(CR )  ALPHA(TI )  ALPHA(P2 )  ALPHA(S2 )  ALPHA(SI )
    1.49500*    5.92900*    1.61300*    2.23000*    1.22600*

FILE:STLR50,1(22-03-1979)
DATE:22-03-1979 15.06
```

Start regression analysis shows satisfactory results

```
* PRL
NR INTENSITY ---------CONCENTRATION---------   APPARENT CONCENTR. IDENTIFICATION
             CHEMICAL  CALCULATED    DIFF.    CHEMICAL  CALCULATED
 1   0.923   15.20000   15.23826   0.03826   11.81437   11.84410 SS-61
 2   0.769   12.80000   12.89799   0.09799    9.84635    9.92173 SS-62
 3   1.068   18.70000   18.63349  -0.06651   13.70531   13.65656 SS-63
 4   1.304   25.60000   25.77364   0.17364   16.48265   16.59445 SS-64
 5   1.033   18.45000   18.39801  -0.05199   13.25308   13.21573 SS-65
 6   0.943   17.60000   17.54050  -0.05950   12.12912   12.08811 SS-66
 7   0.999   17.80000   17.81247   0.01247   12.77656   12.78551 SS-67
 8   1.044   18.55000   18.40187  -0.14813   13.45755   13.35008 SS-68
```

Print results list

```
* SRR 50
NDEC=    3 := 2
```

Save regression results (to CP list 50)
Number of decimals in readout

Fig. 2.5L Alpha factors input.

A sample can be excluded from the regression calculation by giving DSA, see figure 2.5M. Note that it is deleted for the regression calculations only, and the data remain in the computer memory and on the disc. One sample can be deleted by giving the sample number in the argument. If a range of samples are to be deleted this range must be specified by two arguments (e.g. DSA 1 6 deletes samples 1 to 6).
Deleted samples are marked in the PRL-list with an asterisk.
If only a few of the samples are to be used in the regression, it may be easier to delete all samples first (by DSA without argument) and then insert the required samples again.

Samples can be inserted again by ISA. If no argument is given all samples are inserted again. One sample can be inserted by giving the sample number in the argument; a range of samples is inserted by giving two arguments.

If samples are deleted for the regression of one element they will also remain deleted for next elements after NRE unless inserted again.

```
* SRA                                        Start regression analysis
ELEMENT= CR       MODEL= DJ     SIGMA=    0.72824     K=    0.17171

      D              E
   -5.36458      23.18992

FILE:STLR50,1(22-03-1979)
DATE:28-03-1979 16.59

* PRL                                        Print results list
NR INTENSITY ---------CONCENTRATION---------  APPARENT CONCENTR. IDENTIFICATION
             CHEMICAL CALCULATED    DIFF.    CHEMICAL CALCULATED
 1   0.923   15.20000   16.04499  0.84499    15.20000   16.04499 SS-61
 2   0.769   12.80000   12.47494 -0.32506    12.80000   12.47494 SS-62
 3   1.068   18.70000   19.41091  0.71091    18.70000   19.41091 SS-63
 4   1.304   25.60000   24.86687 -0.73313    25.60000   24.86687 SS-64
 5   1.033   18.45000   18.59224  0.14224    18.45000   18.59224 SS-65
 6   0.943   17.60000   16.49813 -1.10187    17.60000   16.49813 SS-66
 7   0.999   17.80000   17.79328 -0.00672    17.80000   17.79328 SS-67
 8   1.044   18.55000   18.84174  0.29174    18.55000   18.84174 SS-68

* DSA 6                                     Sample 6 deleted


* SRA
ELEMENT= CR       MODEL= DJ     SIGMA=    0.59146     K=    0.13964

      D              E
   -5.87532      23.54744

FILE:STLR50,1(22-03-1979)
DATE:28-03-1979 16.59

* PRL
NR INTENSITY ---------CONCENTRATION---------  APPARENT CONCENTR. IDENTIFICATION
             CHEMICAL CALCULATED    DIFF.    CHEMICAL CALCULATED
 1   0.923   15.20000   15.86432  0.66432    15.20000   15.86432 SS-61
 2   0.769   12.80000   12.23923 -0.56077    12.80000   12.23923 SS-62
 3   1.068   18.70000   19.28214  0.58214    18.70000   19.28214 SS-63
 4   1.304   25.60000   24.82222 -0.77778    25.60000   24.82222 SS-64
 5   1.033   18.45000   18.45084  0.00084    18.45000   18.45084 SS-65
6*   0.943   17.60000   16.32445 -1.27555    17.60000   16.32445 SS-66
 7   0.999   17.80000   17.63956 -0.16043    17.80000   17.63956 SS-67
 8   1.044   18.55000   18.70419  0.15419    18.55000   18.70419 SS-68

* ISA                                       Insert all deleted samples.
```

Fig. 2.5M Deletion of samples from the calcualtion

If an error is made during the input of concentration or intensity data, correction is possible using the CCD (correct concentration data), or the CID (correct intensity data) commands. The format of the arguments to the commands depends on the regression calculation model which has been chosen. Note that by using CCD and CID the data are corrected in the computer memory only, not in the file on disc. For correction of the data in the file on disc see CHC and CHI (fig. 2.7G).
For the DJ and RH models the element must be specified with CCD, but not with CID. For the LP model the element must be specified with CID, but not with CCD, refer to the listing of commands in paragraph 2.2.

```
* SRA
ELEMENT= TI       MODEL= DJ     SIGMA=    0.18271     K=    0.24712

      D             E       ALPHA(MO )  ALPHA(NB )  ALPHA(NI )  ALPHA(MN )
    0.01369     -0.00879     3.06500*    2.85600*    0.26500*   -0.11500*

 ALPHA(CR )  ALPHA(TI )  ALPHA(P2 )  ALPHA(S2 )  ALPHA(SI )
   -0.20000*    1.00500*    0.99000*    1.45600*    0.70000*

FILE:STLR50,1(22-03-1979)
DATE:22-03-1979 14.39

* PRL
NR INTENSITY -------CONCENTRATION--------  APPARENT CONCENTR. IDENTIFICATION
             CHEMICAL CALCULATED   DIFF.   CHEMICAL CALCULATED
 1   0.018   0.00000   0.01339  0.01339    0.00000   0.01353 SS-61
 2   0.017   0.00000   0.01370  0.01370    0.00000   0.01355 SS-62
 3   0.017   0.00000   0.01342  0.01342    0.00000   0.01354 SS-63
 4   0.021   0.46000   0.01366 -0.44634    0.45497   0.01351 SS-64
 5   1.346   0.00200   0.00185 -0.00015    0.00201   0.00186 SS-65
 6   0.037   0.00200   0.01428  0.01228    0.00187   0.01337 SS-66
 7   0.028   0.00000   0.01375  0.01375    0.00000   0.01344 SS-67
 8   0.024   0.00000   0.01344  0.01344    0.00000   0.01348 SS-68

* CCD 4 TI                          Correct concentration of Ti in sample 4.
   0.46000 := 0                     New value input


* CCD 5 TI                          Correction of sample 5.
   0.00200 := .46


* SRA                               Regression analysis with new values.
ELEMENT= TI       MODEL= DJ     SIGMA=    0.00207     K=    0.00652

      D             E       ALPHA(MO )  ALPHA(NB )  ALPHA(NI )  ALPHA(MN )
   -0.00787     0.34789     3.06500*    2.85600*    0.26500*   -0.11500*

 ALPHA(CR )  ALPHA(TI )  ALPHA(P2 )  ALPHA(S2 )  ALPHA(SI )
   -0.20000*    1.00500*    0.99000*    1.45600*    0.70000*

FILE:STLR50,1(22-03-1979)
DATE:22-03-1979 14.42

* PRL                               Print results list output shows changed values.
NR INTENSITY -------CONCENTRATION--------  APPARENT CONCENTR. IDENTIFICATION
             CHEMICAL CALCULATED   DIFF.   CHEMICAL CALCULATED
 1   0.018   0.00000  -0.00152 -0.00152    0.00187   0.00051 SS-65
 2   0.017   0.00000   0.00321  0.00321    0.00187   0.00488 SS-66
 7   0.028   0.00000   0.00208  0.00208    0.00000   0.00204 SS-67
 8   0.024   0.00000   0.00062  0.00062    0.00000   0.00062 SS-68

* SRR 50
NDEC=   3 := 2
```

Fig. 2.5N Correction of input data

Regression analysis using the Rasberry-Heinrich model

This procedure is basically the same as for the DJ model, but note that an inter-element correction cannot include both an alpha and a beta constant for the same correction element. The alpha constant is intended to correct for absorption effects, and the beta for enhancement effects, and an alpha or beta value should be input in the regression procedure dependent on which effect is predominant. A regression analysis using the R-H model is shown in figure 2.5P.

```
* SRI                                        Start regression input
MODEL= DJ :=RH                              Change to Rasberry—Heinrich calculation model
LOAD ALL ELEMENTS =YE:=                     Load all element data from the STL file
LOADED ELEMENTS:   MO     NB     NI     MN     CR     TI     P2     S2     SI

  8 OF THE   8 SAMPLES LOADED
REGR. ELMNT :=CR                            Element chosen for regression analysis is chromium

* CAL MO                                    Calculate alpha constant Cr/Mo

* CBT NI                                    Calculate beta constant Cr/Ni

* SRA                                       Start regression analysis routine
ELEMENT= CR       MODEL= RH     SIGMA=    0.29214     K=    0.06962

      D            E        ALPHA(MO )    BETA(NI )     Results showing D, E, α (Cr/Mo)
   -3.88169     20.21780      3.68810      0.87150      and β (Cr/Ni) constants.

FILE:STLR50,1(22-03-1979)
DATE:22-03-1979 16.19

* PRL                                       Print results list
NR INTENSITY ------CONCENTRATION---------  APPARENT CONCENTR. IDENTIFICATI(
           CHEMICAL CALCULATED   DIFF.    CHEMICAL CALCULATED
 1   0.923 15.20000  15.49389  0.29389    14.50352  14.78394 SS-61
 2   0.769 12.80000  12.80272  0.00272    11.66897  11.67144 SS-62
 3   1.068 18.70000  18.96413  0.26413    17.47170  17.71848 SS-63
 4   1.304 25.60000  25.69931  0.09931    22.38833  22.47518 SS-64
 5   1.033 18.45000  18.20898 -0.24102    17.22981  17.00473 SS-65
 6   0.943 17.60000  17.60574  0.00574    15.17406  15.17901 SS-66
 7   0.999 17.80000  17.48141 -0.31859    16.60537  16.30816 SS-67
 8   1.044 18.55000  18.42445 -0.12555    17.33961  17.22225 SS-68

*
```

Figure 2.5P Example of the R—H calculation model.

2.5.3. Results to calculation parameters list (CP-list).

When the results are acceptable, after the operations described in paragraph 2.5.2., they can be transferred to the designated CP list using the command SRR.
The sequence order of the SRR element transfer to the CP list will determine the order of readout of the concentration results from sample measurement.

The SRR command will require an argument to define the CP list number, which is often the same as the MP/LP list numbers, see figure 2.5Q.

The first time that the element parameters are saved by SRR, the identification name of the CP list is requested (as in ACP), and the number of decimals in the readout of sample measurement results must be defined (maximum of five decimals). When the SRR command is given for succeeding elements only the number of decimals must be input.

```
*!SRA !                                        Start regression analysis
ELEMENT= SI       MODEL= DJ     SIGMA=    0.00747     K=    0.00971

      D             E       ALPHA(MO )  ALPHA(NB )  ALPHA(NI )  ALPHA(MN )
   -0.05217      1.30101     -0.34900*   -0.39300*    0.26500*   -0.11600*

 ALPHA(CR )  ALPHA(TI )  ALPHA(P2 )  ALPHA(S2 )  ALPHA(SI )
   -0.21400*   -0.64300*   -0.84500*   -0.81200*   -0.79800*

FILE:STLR50,1(22-03-1979)
DATE:22-03-1979 13.51

* PRL                                          Print results list (now satisfactory)
NR  INTENSITY -------CONCENTRATION--------  APPARENT CONCENTR. IDENTIFICATION
            CHEMICAL  CALCULATED    DIFF.  CHEMICAL  CALCULATED
 1    0.370   0.42000   0.42014  0.00014   0.42880    0.42895 SS-61
 2    0.369   0.44000   0.42864 -0.01136   0.43970    0.42834 SS-62
 3    0.389   0.45000   0.44433 -0.00567   0.45907    0.45329 SS-63
 4    0.391   0.45000   0.45288  0.00288   0.45366    0.45656 SS-64
 5    0.567   0.67000   0.67086  0.00086   0.68459    0.68546 SS-65
 6    0.450   0.51000   0.51917  0.00917   0.52384    0.53326 SS-66
 7    0.439   0.50000   0.50782  0.00782   0.51140    0.51940 SS-67
 8    1.160   1.42000   1.41563 -0.00437   1.46199    1.45749 SS-68

* SRR 50                                     Save (and transfer) constants for Si to CP list 50
NEW LIST
NAME =                                  := STAINLESS STEELS   Identification
NDEC=    3 := 2                         Number of decimals to be given   (first time only)
                                        in results readout
```

Fig. 2.5Q. Constants saved to CP list.

Note that the maximum number of matrix corrections that can be saved in CP list is 189.

Following the transfer of the constants to the CP list (for the first element in the regression analysis routine) the next element for analysis can be selected by giving command NRE (next regression element, see fig. 2.5R).

Note that previously input interelement correction factors are reset (in the same way as RCF), but samples deleted by DSA will remain deleted for the following analysis. If required, reinsert the stored sample intensity/concentration values for regression analysis by giving ISA.

```
* NRE                                    Next regression element
REGR.ELMNT ;= CR                        Choose element for analysis

* SRA                                    Start regression analysis
ELEMENT= CR     MODEL= DJ    SIGMA=    0.72824    K=    0.17171

     D              E
  -5.36458      23.18992

FILE:STLR50,1(22-03-1979)
DATE:22-03-1979 15.03

                                        Regression analysis to follow previous element procedure
```

Fig. 2.5R. Next element for regression analysis.

2.6. INSTRUMENT RECALIBRATION

The DJ and RH concentration calculation models separate the constants related to the instrument (D and E), from those which are dependent on the sample (the component containing alphas and possibly betas), see paragraph 2.1.3. If major items are changed in the spectrometer system (such as the X-ray tube), or drift is experienced or suspected, it may be necessary to check and update the instrument dependent constants D and E. If monitor measurement is used, the stored monitor measurement results must be updated first, see paragraph 2.4.3., but this is not shown in the following examples.

Periodic updating of the D and E constants, for each element used in concentration calculation, can be performed by one of the following methods:

SMR — **manual input;** a set of known calibration samples are measured, and the values of **apparent** concentration are typed in. New values of D and E are calculated, and these can be saved to automatically update the associated CP list. The disc file obtained from this procedure is used during the following two methods. See paragraph 2.6.3.

SSR — **semi-automatic;** after the measurement of the known calibration samples the new D and E values are printed, and these can be saved to update the CP list. See paragraph 2.6.4.

SAR — **automatic;** after measuring the calibration samples, the computer will automatically update the stored D and E constants. See paragraph 2.6.5.

Special samples are kept specifically for instrument recalibrations, and a sufficient number should be loaded for the calculation of the D and E constants for the required elements. The number of samples can be selected by the operator dependent on the precision of recalibration required, and the time available for the recalibration routine.

The "apparent concentration" values used in the recalibration routines can be obtained by the direct measurement of the recalibration standard samples - see paragraph 2.6.2., or by using the results of measuring the calibration standard samples from the regression analysis routine — see paragraph 2.6.1.

2.6.1. Recalibration using regression analysis results

During the regression analysis routine the PRL command output will show a listing of calculated apparent concentrations, for example as figure 2.5Q. If some of these calibration standards are also used in the recalibration routine the values of **calculated apparent concentration** can be used as input for the following recalibration methods.

2.6.2. Standard samples measurement

The measurement of recalibration standard samples uses the SMA i (j) (k) command, where i (j) and (k) are MP/LP lists. With this command the measurement results readout will show a listing of the **apparent concentrations,** see figure 2.6A. Note that the system disc must be in station 0.

```
* SMA 50
SAM.POS= 1 1
IDENT 1= RECAL IDR. STAND. #1


*
  MP 50  CP 50  STAINLESS STEELS
APPARENT CONCENTR. RECALIBR. STAND. #1                    22-03-1979 15.21

SI         MN         S          P          NI         CR         MO
0.82       0.75    0.022      0.013         6.41       6.91       0.02

 NB         TI
-0.02       0.04
```

Fig. 2.6A. Apparent concentrations readout from standard sample measurement.

2.6.3. Manual recalibration

With the SMR command a recalibration file is created in which the details of the calibration procedure are defined, and which can be used later for semi-automatic (SSR) or automatic (SAR) recalibration. A "files" disc must be in station 1 and the AN system disc in station 0.

When the WDD command is given a file identification must also be input, and the system will add a file name extension B followed by the measurement program number, refer to figure 2.6B.
Note that the file identification can be the same as the regression analysis file, as shown in the example.
When the SMR command is given the disc file and extension identification are printed, and the dialog requests input of the sample turret loading and sample identification details. The measurement of the samples commences, to be followed by a readout of the intensities results for each sample.

After all samples have been measured the system requests an input of the apparent concentration values.

The values are obtained from the PRL list in the regression procedure - see paragraph 2.6.1., or from the measurement of standard samples using SMA - see paragraph 2.6.2.

The routine now calculates a best fit for a calibration line through the intensity/apparent concentration values. The intercept and slope values are calculated, and the printout shows the old values (from the CP list) and the newly calculated values. The operator is requested to accept (with c.r.) or refuse (with NO) the values, and if accepted the CP list values are automatically updated.

The above procedure is stored in the file specified by the WDD command, and they can be called for use in the SSR as SAR routines.

```
* WDD DX1:STEELS                          Write data to disc in station 1, with identification STEELS.

* SMR 50                                  Start manual recalibration
RECALIBRATION FILE : DX1:STEELS.B50

NR OF SAMPLES :=  5                       Total of 5 recalibration standards to be used.
SAM.POS= 1 2 3 4 1
IDENT OF S  1 = SS-64                     Loading and identification (first 4 samples).
IDENT OF S  2 = SS-65
IDENT OF S  3 = SS-66
IDENT OF S  4 = SS-67

*
  MF 50  CP 50  STAINLESS STEELS                                  22-MAR-79 16:13
INTENSITIES        SS-64

      MO          NB          NI          MN          CR          TI          P2
 0.02929     0.15621     2.43793     1.63029     1.30457     0.01908     0.47548

      S2         SIO2
 2.21490     0.38065

DATA TO FILE DX1:STEELS.B50

INTENSITIES        SS-65

      MO          NB          NI          MN          CR          TI          P2
 0.07158     0.16712     1.01651     1.63418     1.03230     1.34622     0.82436
```

Fig. 2.6B. Manual recalibration (page 1 of 2).

```
IDENT OF S  5 = SS-68

*          SMR example (continued)                    Loading and identification of fifth sample.
  MP 50  CP 50  STAINLESS STEELS                                  22-03-1979 16.21
INTENSITIES         SS-68

      MO          NB          NI          MN          CR          TI          P2
   0.06951     0.15934     1.00619     2.66951     1.04417     0.02518     1.11366

      S2          SI
   2.49542     1.15468

DATA TO FILE STLB50,1


RECALIBRATION OF MO                    Recalibration of both or only one constant
D = YE :=
E = YE :=
USE ALL SAMPLES = YE :=                Select one or more samples
APPARENT CONCENTRATIONS:


S 1 := .0179
S 2 := .03493
S 3 := 2.46656                         Input value from SMA or regression measurement results.
S 4 := .03473
S 5 := .03751

ELM  S1 S2     D(NEW)      D(OLD)      E(NEW)      E(OLD)
MO    0  0    0.00238    -0.00061     0.43749     0.43359  SAVE=YE :=
                                                           Save to update CP
RECALIBRATION OF NB                                        list (give c.r.) or use
D = YE :=                                                  old value (give NO)
E = YE :=
USE ALL SAMPLES = YE :=
APPARENT CONCENTRATIONS:

S 1 := -.00313
S 2 := .00527
S 3 := .00523
S 4 := 1.03785
S 5 := .00158

ELM  S1 S2     D(NEW)      D(OLD)      E(NEW)      E(OLD)
NB    0  0   -0.12369    -0.12330     0.77414     0.77359  SAVE=YE :=

RECALIBRATION OF NI
D = YE :=
E = YE :=
USE ALL SAMPLES = YE :=

APPARENT CONCENTRATIONS:
S 1 := 25.40969
S 2 := 10.53249
S 3 := 10.66006
S 4 := 10.46544
S 5 := 10.44632
ELM  S1 S2     D(NEW)      D(OLD)      E(NEW)      E(OLD)
NI    0  0   -0.12984    -0.15610    10.47550    10.50491  SAVE=YE :=
```

Fig. 2.6B. Manual recalibration (page 2 of 2).

continued for all elements.

2.6.4. Semi-automatic recalibration

Semi-automatic recalibration is initiated by the SSR command, but only after manual calibration has been carried out as paragraph 2.6.3. and the recalibration file is present on the "files" disc, and after the WDD command is given to gain access to this file.

When SSR is given the recalibration samples must be loaded when the identification is printed, and measurement commences. After the results readout the new values for constants D and E are automatically calculated and printed, and for each element the operator can accept or refuse to save the constants and update the CP list, see figure 2.6C.

```
* WDD STL,1                                        Write data to disc

* SSR 50                                           Start recalibration
RECALIBRATION FILE : STLB50,1
GIVE CR AFTER LOADING S  1 : SS-64
GIVE CR AFTER LOADING S  2 : SS-65                 Load samples and give c.r.
GIVE CR AFTER LOADING S  3 : SS-66
GIVE CR AFTER LOADING S  4 : SS-67

*                                                  Measurement results
  MF 50  CP 50  STAINLESS STEELS                                22-03-1979 17.08
INTENSITIES        SS-64

     MO          NB          NI          MN          CR          TI          P2
  0.03436     0.15859     2.43781     1.65087     1.30146     0.01941     0.51895

     S2          SI
  2.30510     0.38400

DATA TO FILE STLB50,1

                                                   Continue for all samples
                                                   Final sample results

     MO          NB          NI          MN          CR          TI          P2
  0.07544     0.15423     1.00600     2.65946     1.04413     0.02398     0.96801

     S2          SI
  2.52382     1.14952

DATA TO FILE STLB50,1

ELM   S1 S2      D(NEW)      D(OLD)      E(NEW)      E(OLD)
MO     0  0     0.00259     0.00238     0.43996     0.43749  SAVE=YE :=
NB     0  0    -0.12385    -0.12369     0.77983     0.77414  SAVE=YE :=
NI     0  0    -0.11330    -0.12984    10.46955    10.47550  SAVE=YE :=
MN     0  0    -0.10643    -0.10007     0.61735     0.61392  SAVE=YE :=
CR     0  0     0.08134     0.25362    12.69978    12.53395  SAVE=YE :=   Give c.r. or NO
TI     0  0    -0.00767    -0.00775     0.34721     0.34782  SAVE=YE :=
P2     0  0     0.00385     0.00492     0.01902     0.01674  SAVE=YE :=
S2     0  0     0.00866     0.00795     0.00635     0.00687  SAVE=YE :=
SI     0  0    -0.05183    -0.04568     1.31046     1.29770  SAVE=YE :=
```

Fig. 2.6C. Semi-automatic recalibration.

*

2.6.5. Automatic recalibration

The automatic recalibration procedure is similar to SSR, but constants are automatically saved to the CP list. Give WDD before SAR.

```
* WDD STL,1

* SAR 50;                                          Start automatic recalibration
RECALIBRATION FILE : STLB50,1
GIVE CR AFTER LOADING S  1 : SS-64
GIVE CR AFTER LOADING S  2 : SS-65                 Load samples and give c.r.
GIVE CR AFTER LOADING S  3 : SS-66
GIVE CR AFTER LOADING S  4 : SS-67

*
  MP 50  CP 50  STAINLESS STEELS                          22-03-1979 17.35
INTENSITIES        SS-64

      MO          NB          NI          MN          CR          TI          P2
   0.03713     0.15186     2.43781     1.63760     1.30508     0.01914     0.53168

      S2          SI
   2.17231     0.38517

DATA TO FILE STLB50,1

INTENSITIES        SS-65

      MO          NB          NI          MN          CR          TI          P2
   0.08512     0.16119     1.01521     1.64186     1.03250     1.34211     0.84048

      S2          SI
   2.56681     0.57001

DATA TO FILE STLB50,1
*                          ————————  Continue for all samples  ————————
  MP 50  CP 50  STAINLESS STEELS                          22-03-1979 17.41
INTENSITIES        SS-68

      MO          NB          NI          MN          CR          TI          P2
   0.08654     0.15623     1.00600     2.64371     1.04541     0.02441     1.00101

      S2          SI
   2.49607     1.15419

DATA TO FILE STLB50,1

ELM   S1 S2      D(NEW)      D(OLD)      E(NEW)      E(OLD)
MO     0  0    -0.00120     0.00259     0.43966     0.43996
NB     0  0    -0.11945    -0.12385     0.77009     0.77983
NI     0  0    -0.11274    -0.11330    10.46895    10.46955
MN     0  0    -0.11873    -0.10643     0.62689     0.61735     New values saved
CR     0  0     0.26810     0.08134    12.51584    12.69978     automatically in
TI     0  0    -0.00777    -0.00767     0.34889     0.34721     CP list.
P2     0  0     0.00418     0.00385     0.01877     0.01902
S2     0  0     0.00721     0.00866     0.00714     0.00635
SI     0  0    -0.05001    -0.05183     1.30247     1.31046

*
```

Fig. 2.6D. Automatic recalibration

2.7. FILES AND DISC OPERATION

This paragraph covers a number of procedures which are not part of the normal sample analysis routine, such as updating disc files, copying discs, etc.
The paragraph information also supplements the notes at the commencement of paragraph 2.1., and the paragraphs 2.1.1. and 2.1.2.

2.7.1. General

The organisation of the X14 software package allows for the provision of a databank file on the systems disc, and this will appear in readouts as PW 1400.DBK. This databank is intended to hold the parameters input to the computer memory, such as link programs, correction and calculation programs, etc. However, it is also possible to store databanks on a "files" disc, in which case the initially empty databank file on the systems disc should be copied to the files disc by giving WDB. Now give the command LDB, and lists which are assembled to the computer memory are immediately transferred to the opened file, i.e. the databank file in the files disc.

When all the required lists have been assembled and stored, the parameter bank which is in the microprocessor part can also be stored in the files disc, by giving the DPB command. This extension to the X14 file is identified by PB. Thus, all the relevant analysis programs can be safely stored, and for extra security the file can be copied to another disc, see paragraph 2.7.2.

For general information the commands associated with the parameter bank and databank operation are listed below:

Microprocessor commands (C=)

PPB — Print the parameter bank contents
PPB a — Print a specified part (a) of the parameter bank
DPB — Dump the parameter bank
RPB — Read in the parameter bank
CPB — Clear the parameter bank (to zero data)

X14 software (*)

WDB — Write databank from the computer memory to disc, with a specified identification
LDB — Load the specified databank from disc into the computer memory.

DEC PDP11 Software (.)

DIR — Readout the file reference, size, and date, stored on the disc in a specified station.
@Copy — Copy the contents of the disc loaded in station 0 to the disc in station 1. Can only be used to copy system discs.
COPY — Copy a specified file from the disc in one station to the disc in the other station.
DEL — Delete a specified file from the disc in the specified station.
INIT — Initiate a disc in the specified station.

2.7.2. Copy entire discs

It is recommended that when the PW 1400 system is first used the system disc is copied, and the master disc can then be kept in a safe place so that further copies can be made when the first copy disc is worn. It may also be necessary to reproduce the files disc data - see paragraph 2.7.3. Note that @COPY can only be used if the system disc used has the COPY.COM and COPYTX.LST routines.

Proceed as follows:

- Load the system (or master) disc in station 0 (DX0), and the new disc in station 1 (DX1).
- Type @COPY, where @ is the Decwriter upper case 2.
- Answer Y to the request "Init are you sure ?", see figure 2.7A 1.
  The entire contents of the disc in station 0 is written to the disc in station 1, and any data on the latter disc will be overwritten.

```
.@COPY

.COPY/DEVICE SY0: SY1:

SY1:/Copy are you sure?Y

.TYPE X14D20.HED


S Y S T E M S D I S K E T T E     X 1 4 D - S O F T W A R E


V E R S I O N   2 . 0



.DIR/VOLUME/C:2/ORDER:NAME DX1:
 29-Oct-79
 Volume ID: 402215184621
 Owner    : N.V. PHILIPS
COPY   .COM      1 06-Sep-79       RESORC.SAV     12 11-Mar-78
DIR    .SAV     17 11-Mar-78       RT     .SYS     2 07-Jun-79
DUP    .SAV     21 24-Mar-78       STARTS.COM      1 15-Oct-79
DXMNSJ.SYS      61 07-Jun-79       SWAP   .SYS    24 11-Mar-78
LP     .SYS      2 30-Dec-78       SYSPAR.DAT      1 18-Sep-79
PIP    .SAV     16 11-Mar-78       TT     .SYS     2 07-Jun-79
PW1400.DBK       3 21-Dec-79       X14D20.HED      1 22-Aug-79
PW1400.SAV     275 15-Oct-79
 15 Files, 439 Blocks
 41 Free blocks
```

Fig. 2.7A1. Copy disc routine.

Initiating a new disc

A disc must be initiated before it can be used to record files. This can be done by the @COPY command as above, or by the INIT command, see figure 2.7A2. In both cases any existing data on the new disc will be erased. Proceed as follows:

- Place the system disc in station 0, and the new disc in station 1.
- Type INIT/BADBLOCKS DX1:
- Answer 'Y' to request "Init are you sure? ":

A dot will be printed when the routine is complete

```
.INIT/BADBLOCKS DX1:

DX1:/Init are you sure?Y
```

Fig. 2.7A2. Initiation a new disc.

2.7.3. Copy files

To copy specified files from one disc to another disc the dot mode copy routine is used, as shown in figure 2.7A3. The format is from disc station: file reference, to disc station: file reference. Note that an asterisk can be used to denote all files or file extensions, or copied file name to be the same as the original.

```
.COPY DX0:DB1400.DBK DX1:DB1400.DBK
```
Copy databank from disc 0 to 1

```
.COPY DX0:DB1400.PBK DX1:*.*
 Files copied:
DX0:DB1400.PBK to DX1:DB1400.PBK
```
Copy same parameter bank name

Readout after copy completed

```
.COPY DX0:STEELS.* DX1:*.*
 Files copied:
DX0:STEELS.R50 to DX1:STEELS.R50
DX0:STEELS.B50 to DX1:STEELS.B50
DX0:STEELS.C50 to DX1:STEELS.C50
.
```
Copy all file extensions and give the same name to the copies.

Fig. 2.7A3. Copy disc files.

Delete files

Using a similar format to the above, any file can be deleted from a disc in station 0 or 1. Note that all dot mode deletions require an answer "Y" before a deletion routine is executed, see figure 2.7A4.

```
.DEL DX0:DB1400.DBK
 Files deleted:
DX0:DB1400.DBK? Y
```

```
.DEL DX0:DB1400.*
 Files deleted:
DX0:DB1400.PBK? Y
```
Delete all DB1400 files (only one in this case)

```
.DEL DX0:STEELS.*
 Files deleted:
DX0:STEELS.R50? Y
DX0:STEELS.B50? Y
DX0:STEELS.C50? Y
```
Delete all STEELS files

STEELS file extensions deleted

```
.
```

Fig. 2.7A4. Deletion of disc files.

2.7.4. Update files procedure

Various commands are available to print, correct, delete and add data which is on a files disc, using the UP disc. Access to a file which is to be modified is obtained from the OPF command, which must state the file identification and the disc drive station 0 or 1, if required. When the required modifications have been input the file is closed by giving CLF.

The following routines can be used:

OPF — open the designated file
CLF — close the file

Concentrations — Regression and Recalibration files

ACD — to add concentrations data to a regression intensities file (from SPR command).
PCI — print sample concentrations and intensities from a regression or calibration file.
PID — print intensities only from the file.
PCD — print concentrations only from the file.
Note that a file which has been created by SMX, using a CP list = 0 in the LP list, can have a readout from PCD, although the data are not strictly concentrations.
PSI — print a list of sample identifications.
DLC — delete channel (elements) from the opened file.
ADC — add channel (elements) to the opened file.
DLS — delete sample from the file.
ADS — add sample data to the file.
CHC — change concentration data in the file.
CHI — change intensity data in the file.

Job files

PJF — print of file input from WDD.
PLS — plot of step scan contained in a job file.

Examples

OPF and CLF, see figure 2.7B.
The OPF output will depend on type of file, i.e. the mode designation (C = concentrations, R = regression, B = recalibration, A, B, C, etc. = job).
Give the close file command (CLF) as soon as the readouts or modifications are finished.

Concentration file (SMX)

```
* OPF DX1:STATIS.C03
   90 RECORDS OF LENGTH:  17,  51 EMPTY RECORDS. FILE DATE:28-MAR-79
MODE= 1  MP=  3  CP=  0    38 SAMPLES
  3 CHANNELS: NI    FE    CR
            400.0 100.0 400.0
```

Regression file (SPR)

```
* OPF DX1:STEELS.R50
   16 RECORDS OF LENGTH:  47,   7 EMPTY RECORDS. FILE DATE:22-MAR-79
MODE= 3  MP= 50  CP= 50     8 SAMPLES
  9 CHANNELS: MO    NB    NI    MN    CR    TI    P2    S2    SI
```

Recalibration file (SMR)

```
* OPF DX1:STEELS.B50
   16 RECORDS OF LENGTH:  47,  10 EMPTY RECORDS. FILE DATE:22-MAR-79
MODE= 5  MP= 50  CP= 50     5 SAMPLES
  9 CHANNELS: MO    NB    NI    MN    CR    TI    P2    S2    SI
              0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
              D  E  D  E  D  E  D  E  D  E  D  E  D  E  D  E  D  E
```

Job file (SJB)

```
* OPF DX1:SPECIR.54A
  128 RECORDS OF LENGTH:   6,  65 EMPTY RECORDS. FILE DATE:28-MAR-79
MODE= 8  JOBNR= 54     0 CYCLES
```

Fig. 2.7B. Open file commands.

ACD - see figure 2.7C.

To add concentration data to a regression intensities file opened with OPF. Element concentrations must be input.

```
* OPF STLR50,1                          Open regression file
   18 RECORDS OF LENGTH: 65,   9 EMPTY RECORDS. FILE DATE:22-03-1979
MODE= 3  MP= 50  CP= 50     8 SAMPLES
  9 CHANNELS: MO    NB    NI    MN    CR    TI    P2    S2    SI

* ACD                                  Add concentrations data

SAMPLE  1  SS-61
MO    := .018
NB    := .000
NI    := 6.26
MN    := .78
CR    := 15.2
TI    := .000
P2    := .016
S2    := .016
SI    := .42

SAMPLE  2  SS-62
MO    := .02
NB    := .028
NI    := 12.45
MN    := .8
CR    := 12.8
TI    := .000
P2    := .015
S2    := .02
SI    := .44

SAMPLE  3  SS-63
MO    := .017
NB    := .005
NI    := 9.49
MN    := .79
CR    := 18.7
TI    :=
P2    := .016
S2    := .02
SI    := .45

SAMPLE  4  SS-64
MO    := .014
NB    :=
NI    := 20.6
MN    := .85
CR    := 25.6
TI    := .46
P2    :=
S2
```

Concentrations data input - normally from certified calibration measurement.

and continued for all samples.

Fig. 2.7C. Concentration values added to file

PSI - see figure 2.7D

Identifications of the samples in an opened file are listed.

```
* OPF STLR50,1          Open regression file
   18 RECORDS OF LENGTH: 65,   9 EMPTY RECORDS. FILE DATE:22-03-1979
MODE= 3  MP= 50  CP= 50     8 SAMPLES
  9 CHANNELS: MO    NB    NI    MN    CR    TI    P2    S2    SI

* PSI                    Print sample identifications
  1 SS-61                2 SS-62                3 SS-63
  4 SS-64                5 SS-65                6 SS-66
  7 SS-67                8 SS-68

*
```

Fig. 2.7D. Listing of sample identifications

PCI, PCD and PID - figures 2.7E and F.

Print of concentration and/or intensity data from regression files, concentration files (PCD only), and recalibration files.

If an argument is not given all samples data will be given, one argument can select a particular sample, or two arguments specify a range of samples.

```
* OPF STLR50,1                Open regression file
   18 RECORDS OF LENGTH: 65,   9 EMPTY RECORDS. FILE DATE:22-03-1979
MODE= 3  MP= 50  CP= 50     8 SAMPLES
  9 CHANNELS: MO    NB    NI    MN    CR    TI    P2    S2    SI

* PCI                    Print concentration and intensity data
CONC/INT  MP 50  CP 50  MD  3  SN  1  SS-61                22-03-1979

     MO        NB        NI        MN        CR        TI        P2
  0.01800   0.00000   6.26000   0.78000  15.20000   0.00000   0.01[illegible]
  0.03421   0.15770   0.66691   1.43867   0.92323   0.01[illegible]

     SI
  0.42000                                                  0.01050   1.40524
  0.36980

CONC/T[illegible]
  0.43933

CONC/INT  MP 50  CP 50  MD  3  SN  8  SS-68                22-03-1979

     MO        NB        NI        MN        CR        TI        P2        S2
  0.03300   0.00000   9.33000   1.59000  18.55000   0.00000   0.02700   0.02800
  0.08792   0.16143   1.00928   2.70226   1.04383   0.02440   1.09797   2.37763

     SI
  1.42000
  1.16038
```

Fig. 2.7E. Print concentration and intensity data

```
* PID        Print intensity data
INT        MP 50  CP 50  MD  3  SN  1  SS-61                    22-03-1979

     MO         NB         NI         MN         CR         TI         P2         S2
  0.03421    0.15770    0.66691    1.43867    0.92323    0.01819    0.69968    1.27439

     SI
  0.36980

INT        MP 50  CP 50  MD  3  SN  2  SS-62                    22-03-1979

     MO         NB         NI         MN         CR         TI         P2         S2
  0.05041    0.19547    1.33249    1.42797    0.76928    0.01659    0.49855    1.68475

     SI
  0.36934

INT        MP 50  CP 50  MD  3  SN  3  SS-63                    22-03-1979
     MO         NB         NI         MN         CR         TI         P2         S2
  0.03860    0.17244    1.01987    1.48324    1.06837    0.01714    0.68910    1.87100

     SI
  0.38851

INT        MP 50  CP 50  MD  3  SN  4  SS-64                    22-03-1979

     MO         NB         NI         MN         CR         TI         P2
  0.04269    0.15534    2.43370    1.67569    1.30365    0.02112    0.45[illegible]    _.30731

     SI
  0.39103

INT        MP 50  CP 50  MD  3  SN  5                           22-03-1979

     MO         NB         [illegible]    MN         CR         TI         P2         S2
  0.08196    0.16[illegible]    .2763    1.40915    0.94277    0.03663    1.21529    2.25580

     [illegible]
     .79

INT        MP 50  CP 50  MD  3  SN  7  SS-67                    22-03-1979

     MO         NB         NI         MN         CR         TI         P2         S2
  0.08149    1.50100    1.01110    1.58462    0.99862    0.02846    0.61050    1.40524

     SI
  0.43933

INT        MP 50  CP 50  MD  3  SN  8  SS-68                    22-03-1979

     MO         NB         NI         MN         CR         TI         P2         S2
  0.08792    0.16143    1.00928    2.70226    1.04383    0.02440    1.09797    2.37763

     SI
  1.16038
```

Fig. 2.7F. Print intensity data.

CHC, CHI - see figure 2.7G.

Correction of intensity and concentration data is possible with CHI and CHC. The first argument has to give the sample number for which correction is required, the second argument has to specify for which element the correction has to be performed.

```
* PCI 1                          Print concentration and intensity data for sample 1
CONC/INT   MP 50   CP 50   MD  3   SN  1   SS-61                    22-03-1979

     MO          NI          MN          CR          P2          S2          SI          TI
  0.01800     6.26000     0.78000    15.20000     0.01600     0.01600     0.42000     0.00000
  0.03421     0.66691     1.43867     0.92323     0.69968     1.27439     0.36980     0.01819

* CHC 1 MO                       Change concentration data for sample 1 element Mo
MO   =   0.01800 := .33333Input new concentration value

* CHI 1 MO                       Change intensity data, also for Mo
MO   =   0.03421 := .77777Input new intensity value

* PCI 1                          Print values, now showing change for Mo
CONC/INT   MP 50   CP 50   MD  3   SN  1   SS-61                    22-03-1979

     MO          NI          MN          CR          P2          S2          SI          TI
  0.33333     6.26000     0.78000    15.20000     0.01600     0.01600     0.42000     0.00000
  0.77777     0.66691     1.43867     0.92323     0.69968     1.27439     0.36980     0.01819
```

Fig. 2.7G. Correction of concentration or intensity data.

DLC, DLS, ADC and ADS - see figures 2.7H and I.

These commands delete/add channel/sample data.

```
* OPE STLR50,1                          Open regression file
   18 RECORDS OF LENGTH:  65,   9 EMPTY RECORDS. FILE DATE:22-03-1979
MODE= 3  MP= 50  CP= 50     8 SAMPLES
  9 CHANNELS: MO    NB    NI    MN    CR    TI    P2    S2    SI

* DLC TI                               Delete channel data for Ti
   18 RECORDS OF LENGTH:  59,   9 EMPTY RECORDS. FILE DATE:28-03-1979
MODE= 3  MP= 50  CP= 50     8 SAMPLES
  8 CHANNELS: MO    NB    NI    MN    CR    P2    S2    SI

* DLC NB                               Delete channel data for Nb
   18 RECORDS OF LENGTH:  53,   9 EMPTY RECORDS. FILE DATE:28-03-1979
MODE= 3  MP= 50  CP= 50     8 SAMPLES
  7 CHANNELS: MO    NI    MN    CR    P2    S2    SI


                                       Now only 7 channels, and length of record = 39 words
* DLS 8
                                       Deletion of sample data
* DLS 7
* DLS6

* FCI                                  Print concentrations/intensity (7 elements, 5 samples)
CONC/INT  MP 50  CP 50  MD  3  SN  1  SS-61                    22-03-1979

     MO         NI         MN         CR         P2         S2         SI
  0.01800    6.26000    0.78000   15.20000    0.01600    0.01600    0.42000
  0.03421    0.66691    1.43867    0.92323    0.69968    1.27439    0.36980

CONC/INT  MP 50  CP 50  MD  3  SN  2  SS-62                    22-03-1979

     MO         NI         MN         CR         P2         S2         SI
  0.02000   12.45000    0.80000   12.80000    0.01500    0.02000    ^ '
  0.05041    1.33249    1.42797    0.76928    0.49855    '                .00851

CONC/INT  MP 50  CP 50  MD  7                                    22-03-1979
                                  -- 04
     MO                 MN         CR         P2         S2         SI
  0.01400   20.60000    0.85000   25.60000    0.01200    0.02200    0.45000
  0.04269    2.43370    1.67569    1.30365    0.45612    2.03435    0.39103

CONC/INT  MP 50  CP 50  MD  3  SN  5  SS-65                    22-03-1979

     MO         NI         MN         CR         P2         S2         SI
  0.03100    9.47000    0.94000   18.45000    0.01800    0.02300    0.67000
  0.08196    1.01748    1.68707    1.03307    0.82288    2.30731    0.56697
```

Fig. 2.7H. Deletion of channel/sample data.

```
* ADC TI
```

Add 4 channel (Ti) to samples in file

```
 SN      CONC., INT.(TI   )
  1 := 0 .01819
  2 := 0 .01659
  3 := 0 .01714
  4 := 0 .02112
  5 := .46 1.34631
```

Input of concentration and intensity values for all samples

```
  18 RECORDS OF LENGTH:  59,  12 EMPTY RECORDS. FILE DATE:28-03-1979
MODE= 3  MP= 50  CP= 50     5 SAMPLES
  8 CHANNELS: MO     NI     MN     CR     P2     S2     SI     TI
```

Now 8 channels, and record = 59 words

```
* ADS SS-66
```

Add a sample to file, with identification SS-66

```
          CONC., INT.
MO     := 2.43 5.69006
NI     := 9.48 1.02963
MN     := .81 1.40915
CR     := 17.6 .94277
P2     := .00\0\2 1.21529
S2     := .023 2.2558
SI     := .51 .44999
TI     := .002 .03663
```

Input of concentration and intensity values for all elements in file

```
* PSI
```

Print sample identifications - now for 6 samples

```
  1 SS-61      2 SS-62      3 SS-63
  4 SS-64      5 SS-65      6 SS-66
```

Figure 2.7I. Addition of channel/sample data.

2.8. EXAMPLES OF ANALYSIS

The following paragraphs show examples of complete analysis routines, for cement measurement with output to include moduli calculation and output showing compound names, for a stainless steel analysis including regression analysis, etc. In paragraph 2.8.3. an example of databank and parameterbank operation is given.

2.8.1. Cement analysis

Measurement program (MP/LP10) for cement analysis is performed as follows:

AMP	measurement program (parameter bank)
PMP	
ALP	link program (databank)
PLP	
AML	moduli list, cement moduli calculations
AMS	moduli set
PMS	
ANM	names list, printout of compound names
PNM	

Regression analysis (if required), not shown in the example

SMX	measurement of unknowns, printout of compound names and cement moduli.

```
*AMP 10
```

Measuring program 10 chosen for cement analysis

```
MASK :  1 :=2
ABS  : YE :=
```

Absolute measurement

```
CHAN    PT    PC
          0   0E0 :=FE 10
          0   0E0 :=CA2 20
          0   0E0 :=K 4
          0   0E0 :=S 10
          0   0E0 :=S+ 10
          0   0E0 :=SI 20
          0   0E0 :=AL 20
          0   0E0 :=MG2- 20
          0   0E0 :=MG2 40
          0   0E0 :=NA 40
          0   0E0 :=NA+ 20
          0   0E0 :=/
```

11 channels chosen - channel assembly not shown.

```
*PMP 10
```

Print MP list 10

```
MP 10

MASK :  2
ABS  : YE

CHAN    PT    PC
FE      10   0E0
CA2     20   0E0
K        4   0E0
S       10   0E0
S+      10   0E0
SI      20   0E0
AL      20   0E0
MG2-    20   0E0
MG2     40   0E0
NA      40   0E0
NA+     20   0E0
```

```
* ALP 10
NEW LIST
NRCH=    0 :=
OPTION=   0 :=
MBNR=   0 :=
INT.RATIO= NO :=
CPNR=   0 := 10
MODLST=   0 := 10

*

* PLP10
LPNR= 10      NRCH=   0      CPNR= 10      MODLST= 10      MBNR=   0
OPTION=   0
```

Assemble link program

Moduli calculation and output (AML10)

Print LP list

```
* AML 10
NEW LIST
NR OF MODULI=   0 := 5
 1=    0 := 1
 2=    0 := 2
 3=    0 := 3
 4=    0 := 4
 5=    0 := 5
```

Assemble moduli list 10

Five moduli sets to be used

Moduli set numbers (to be assembled)

```
* AMS 1
NEW LIST
NAME=        := C3*
NDEC=   -1 := 1
NR OF TERMS IN NUMERATOR   =    0 := 4
NR OF TERMS IN DENOMINATOR=    0 :=

       FACTOR   CHANNEL
N 1=   0.00000        :=4.07 CA2
N 2=   0.00000        :=-7.6 SI
N 3=   0.00000        :=-6.72 AL
N 4=   0.00000        :=-1.43 FE
```

Assemble moduli set number 1

Name of set. Note that it is an external element

$C3^* = 4.07\ Ca\ 2 - 7.6Si - 6.72\ Al - 1.43\ Fe$

```
* AMS 2
NEW LIST
NAME=        := C2*
NDEC=   -1 := 1
NR OF TERMS IN NUMERATOR   =    0 := 2
NR OF TERMS IN DENOMINATOR=    0 :=

       FACTOR   CHANNEL
N 1=   0.00000        :=2.867 SI
N 2=   0.00000        :=-.754 C3*
```

$C2^* = 2.867\ Si - 0.754\ C3^*$ (AMS1)

```
*AMS 3
NEW LIST
NAME=        := CC*
NDEC=  -1 := 1
NR OF TERMS IN NUMERATOR   =    0 := 2
NR OF TERMS IN DENOMINATOR=    0 :=

       FACTOR  CHANNEL
N 1=   0.00000       :=2.65 AL
N 2=   0.00000       :=-1.69 FE
```

CC* = 2.65 Al — 1.69 Fe

```
*AMS 4
NEW LIST
NAME=        := CF*
NDEC=  -1 := 1
NR OF TERMS IN NUMERATOR   =    0 := 1
NR OF TERMS IN DENOMINATOR=    0 :=

       FACTOR  CHANNEL
N 1=   0.00000       :=3.043 FE
```

CF* = 3.043 Fe

```
*AMS 5
NEW LIST
NAME=        := LS*
NDEC=  -1 := 1
NR OF TERMS IN NUMERATOR   =    0 := 1
NR OF TERMS IN DENOMINATOR=    0 := 3

       FACTOR  CHANNEL
N 1=   0.00000       :=100 CA2
D 1=   0.00000       :=2.8 SI
D 2=   0.00000       :=1.2 AL
D 3=   0.00000       :=.65 FE
```

$$LS^* = \frac{100\ Ca\ 2}{2.8\ Si + 1.2\ Al + 0.65\ Fe}$$

Typical print readout

```
*PMS 5
MSNR=  5      NAME= LS*    NDEC=  1

     NUMERATOR          DENOMINATOR
   FACTOR  CHANNEL     FACTOR  CHANNEL
100.00000   CA2       2.80000   SI
                      1.20000   AL
                      0.65000   FE
```

```
* ANM 1
```

Assemble names, from combination 1

```
    ELM,COMPOUND
 1=     ,        := NA,NA2O
 2=     ,        := MG2,MGO
 3=     ,        := AL,AL2O3
 4=     ,        := SI,SIO2
 5=     ,        := S,SO3
 6=     ,        := K,K2O
 7=     ,        := CA2,CAO
 8=     ,        := FE,FE2O3
 9=     ,        := C3,C3S
10=     ,        := C2,C2S
11=     ,        := CC,C3A
12=     ,        := CF,C4AF
13=     ,        := LS,LSF
14=     ,        := /
```

Listing of channel/moduli names

```
* PNM
```

	1	2	3	4	5	6	7	8	9	10
0	NA NA2O	MG2 MGO	AL AL2O3	SI SIO2	S SO3	K K2O	CA2 CAO	FE FE2O3	C3 C3S	C2 C2S
10	CC C3A	CF C4AF	LS LSF							

Sample measurement and results output

Note that calculation parameters list CP10 was assembled by a regression routine — not shown here. Regression analysis is shown in the stainless steel example in paragraph 2.8.2.

```
* SMX 10
SAM,POS= 1 I
IDENT 1= C 2476/27
```

Start measurement of unknown samples
Load sample
Sample identification

Results output showing moduli

```
* MP 10  CP 10  CEMENT ANALYSIS                    22-03-1979 09.55
CONCENTRATIONS     C 2476/27

      CAO      SIO2     AL2O3     FE2O3      SO3       MGO      NA2O
     64.3      21.4       5.5       3.3       2.1       1.7      0.65

      K2O       C3S       C2S       C3A      C4AF       LSF
     0.39      57.4      18.1       9.0      10.0      93.6

*
```

2.8.2. Stainless steel analysis

Measurement program (MP/LP50) for stainless steel analysis, showing:

AMP	PMP		measurement program
ALP	PLP		link program
AMB			monitor buffer
ARC	PRC		countrate correction (line overlap)
LDM	SMM	ULM	monitor measurement
WDD	SPR	NDD	regression intensities
OPF	ACD		regression concentrations
SRI			regression input
SRA			regression analysis
PRL			regression list printed
CCD			correct concentration input error
CAL			calculate alpha
FAL			enter known alpha value
SRR			save regr. results in CP-list
NRE			next regression element
PCP			print CP list made by SRR
LDM	SMM	ULM	monitor update
SMX			measure unknowns, concentrations
PIN			print also gross intensities
WDD	SMR		manual recalibration
NPI			no printing of gross intensities
WDD	SAR		automatic recalibration
PCP			print CP-list from SAR

```
* AMP 50

MASK :  1 :=
ABS  : YE :=N
BRAT : NO :=Y
MOPS :  1 :=
MOMPY:  1 :=2

CHAN    PT   PC
         0  0E0 :=M0 10
         0  0E0 :=M0+  2
         0  0E0 :=NB 10
         0  0E0 :=NI 20
         0  0E0 :=MN 10
         0  0E0 :=CR 20
         0  0E0 :=TI  4
         0  0E0 :=P2 10
         0  0E0 :=P2+  4
         0  0E0 :=S2-  4
         0  0E0 :=S2 10
         0  0E0 :=SI 20
         0  0E0 :=/
```

```
* PMP 50

MP 50

MASK :  1
ABS  : NO
BRAT : YE          Buffer ratio mode
MOPS :  1
MOMPY:  2          Monitor measurement time doubled

CHAN    PT   PC
M0      10  0E0
M0+      2  0E0
NB      10  0E0
NI      20  0E0
MN      10  0E0
CR      20  0E0
TI       4  0E0
P2      10  0E0
P2+      4  0E0
S2-      4  0E0
S2      10  0E0
SI      20  0E0
```

* Channel assembly not shown.

```
* ALP 50
NEW LIST
NRCH=    0 := 2
OPTION=   0 :=
MBNR=   0 := 50
*** MONITORBUFFER 50 DOES NOT EXIST  Warning only
INT.RATIO= NO :=
CPNR=   0 := 50
MODLST=   0 :=

     CHAN RC   A
  1=        0   N   := P2 1
  2=        0   N   := S2 2
```

Assemble link program

Monitor buffer list number

Concentration to use CP50 list parameters

Background and line overlap correction for these channels.

```
* AMB 50
NEW LIST
NRCH=    0 := 9
```

Monitor buffer list (to reserve space in databank)

```
* PLP 50
LPNR= 50      NRCH=   2      CPNR= 50      MODLST=   0      MBNR= 50
OPTION=   0

ELMNT P2    S2
RC      1     2
ABS     N     N
```

Print LP list (for reference).

```
* ARC 1
BKGR=     0 :=
CHL1=       := P2+
L1= 0.0000  := 1
CHL2=       :=
CHL3=       := MO
L3= 0.0000  := .00158
CHL4=       :=
```

Assemble countrate correction set

Background correction parameter

Line overlap correction parameter

```
* ARC 2
BKGR=     0 :=
CHL1=       := S2-
L1= 0.0000  := 1
CHL2=       :=
CHL3=       := MO
L3= 0.0000  := .00541
CHL4=       :=
```

Background

Line overlap

```
* PRC
```

Print (all) RC sets

NR	BKGR	CHL1	L1	CHL2	L2	CHL3	L3	CHL4	L4
1	0	P2+	1.0000		0.0000	MO	0.0016		0.0000
2	0	S2-	1.0000		0.0000	MO	0.0054		0.0000

Now the monitor sample must be measured

```
*!LDM 1 !
```
Load monitor sample in turret position 1

```
*!SMM 50
```
Start monitor measurement

```
*
  MP 50  CP 50  NET INTENSITIES                          22-03-79 12.46

      MO          NB          NI          MN          CR          TI          P2
    3005.       5218.       26837.       1037.       31122.      19306.       35.

      S2          SI
     33.         2266.
```
These results are stored in the monitor buffer so that ratio intensities can be calculated.

```
* ULM 1 !
```
Unload monitor sample (if required)

```
* WDD STL,1
```
Write data to STL file of disc in station 1

```
* SPR 50
SAM.POS= 1 2 3 4 !
IDENT 1= SS-61
IDENT 2= SS-62
IDENT 3= SS-63
IDENT 4= SS-64
```
Load and identify first four standard samples, in turret positions 1 to 4 (batch mode)

```
*
  MP 50  CP 50                                           22-03-1979 13.08
INTENSITIES          SS-61

      MO          NB          NI          MN          CR          TI          P2
   0.03421     0.15770     0.66691     1.43867     0.92323     0.01819     0.69968

      S2          SI
   1.27439     0.36980

DATA TO FILE STLR50,1
```
Above data are stored in STL file, and given a file extension name R50 (R= regression intensities, and 50 = MP list number used).

```
INTENSITIES          SS-62

      MO          NB          NI          MN          CR          TI          P2
   0.05041     0.19547     1.33249     1.42797     0.76928     0.01659     0.49855

      S2          SI
   1.68475     0.36934

DATA TO FILE STLR50,1
```
Data stored for sample 55 - 62

```
INTENSITIES          SS-63

      MO          NB          NI          MN          CR
   0.03860     0.17244     1.01987     1.40734

      S2
   1.[illegible]
```
Similar readout data stored in file STLR50

```
INTENSITIES          SS-64

     MO          NB          NI          MN          CR          TI          P2
0.04269     0.15534     2.43370     1.67569     1.30365     0.02112     0.45612

     S2          SI
2.03435     0.39103

DATA TO FILE STLR50,1

* SPR 50
SAM.POS= 1 2 3 4 I
IDENT 1= SS-65
IDENT 2= SS-66
IDENT 3= SS-67
IDENT 4= SS-68
```

Start prepare regression for the next four samples

```
*
  MP 50  CP 50                                        22-03-1979 13.32

INTENSITIES          SS-65

     MO          NB          NI          MN          CR          TI          P2
0.08196     0.16621     1.01748     1.68707     1.03307     1.34631     0.82288

     S2          SI
2.30731     0.56697

DATA TO FILE STLR50,1

INTENSITIES          SS-66

     MO          NB          NI          MN          CR          TI          P2
5.69006     0.16615     1.02963     1.40915     0.94277     0.03663     1.21529

     S2          SI
2.25580     0.44999

DATA TO FILE STLR50,1

INTENSITIES          SS-67

     MO          NB          NI          MN          CR          TI          P2
0.08149     1.50100     1.01110     1.58462     0.99862     0.02846     0.61050

     S2          SI
1.40524     0.43933

DATA TO FILE STLR50,1

INTENSITIES          SS-68

     MO          NB          NI          MN          CR          TI          P2
0.08792     0.16143     1.00928     2.70226     1.04383     0.02440     1.09797

     S2          SI
2.37763     1.16038

DATA TO FILE STLR5061
```

Repeat procedure until all standard samples are measured.
No data to disc - to reset WDD.

```
* NDD
```

The regression file (STEELS), with the intensity data, is now extended by manual input of concentration data obtained from certified composition figures.

```
* OPF DX1:STEELS.R50        Open regression file STLR50 of disc in station 1.
   16 RECORDS OF LENGTH:   47,    7 EMPTY RECORDS. FILE DATE:22-MAR-79
MODE= 3   MP= 50   CP= 50      8 SAMPLES
  9 CHANNELS: MO     NB     NI     MN     CR     TI     P2     S2     SI

* ACD                        Add the concentration data to the file

SAMPLE   1  SS-61
MO    :=  .018
NB    :=  .000
NI    :=  6.26
MN    :=  .78
CR    :=  15.2
TI    :=  .000
P2    :=  .016
S2    :=  .016
SI    :=  .42

SAMPLE   2  SS-62
MO    :=  .02
NB    :=  .028
NI    :=  12.45
MN    :=  .8
CR    :=  12.8
TI    :=  .000
P2    :=  .015
S2    :=  .02
SI    :=  .44

SAMPLE   3  SS-63
MO    :=  .017
NB    :=  .005
NI    :=  9.49
MN    :=  .79
CR    :=  18.7
TI    :=
P2    :=  .016
S2    :=  .02
SI    :=  .45

SAMPLE   4  SS-64
MO    :=  .014
NB    :=
NI    :=  20.6
MN    :=  .85
CR    :=  25.6
TI    :=  .46
P2    :=  .012
S2    :=  .022
SI    :=  .45
```

Concentration values input for each element of sample

Input repeated for all samples

```
SAMPLE   5  SS-65
MO    :=  .031
NB    :=  .006
NI    :=  9.47
MN    :=  .94
CR    :=  18.45
TI    :=  .002
P2    :=  .018
S2    :=  .023
SI    :=  .67

SAMPLE   6  SS-66
MO    :=  2.43
NB    :=  .006
NI    :=  9.48
MN    :=  .81
CR    :=  17.6
TI    :=  .002
P2    :=  .02
S2    :=  .023
SI    :=  .51

SAMPLE   7  SS-67
MO    :=  .041
NB    :=  1.02
NI    :=  9.53
MN    :=  .87
CR    :=  17.8
TI    :=
P2    :=  .016
S2    :=  .018
SI    :=  .5

SAMPLE   8  SS-68
MO    :=  .033
NB    :=
NI    :=  9.33
MN    :=  1.59
CR    :=  18.55
TI    :=
P2    :=  .027
S2    :=  .028
SI    :=  1.42

* CLF                       Close the file
```

```
* SRI                                  Start regression input (from files disc to the memory)
MODEL= DJ :=                          Select the calculation model - see paragraph 2.1.3.
LOAD ALL ELEMENTS =YE:=
LOADED ELEMENTS:    MO      NB      NI      MN      CR      TI      P2      S2      SI

  8 OF THE    8 SAMPLES LOADED
REGR. ELMNT := SI                     Select first element for regression analysis

* SRA                                  Start regression analysis (for Si).
ELEMENT= SI        MODEL= DJ      SIGMA=     0.01039      K=     0.01358

       D              E
    -0.04110       1.25447            First calculation result

FILE:STEELS.R50(22-MAR-79)
DATE:22-MAR-79 13:48

* FAL SI -.798
* FAL P2 -.845
* FAL S2 -.812
* FAL TI -.643
* FAL CR -.214
* FAL MN -.116
* FAL NI .265
* FAL NB -.393
* FAL MO -.349
```

Input of known (theoretical) alpha constants to improve the calculations of the D and E (instrument) constants, and hence the calculation of unknown sample concentrations.

The second regression analysis below shows an inprovement in the sigma and K values, and this readout also shows alpha values. Alphas which have not been calculated in the regression analysis routine, i.e. not calculated by the CAL command, are designated with an asterisk.
To further improve the results, try the deletion of any sample whose concentration/intensity input is suspect, e.g. if the PRL readout DIFFerence value is high.

```
* SRA                                  Start regression analysis
ELEMENT= SI       MODEL= DJ     SIGMA=    0.00747     K=    0.00971

      D            E       ALPHA(MO )  ALPHA(NB )  ALPHA(NI )  ALPHA(MN )
   -0.05217      1.30101     -0.34900*   -0.39300*    0.26500*   -0.11600*

 ALPHA(CR )  ALPHA(TI )  ALPHA(P2 )  ALPHA(S2 )  ALPHA(SI )
   -0.21400*   -0.64300*   -0.84500*   -0.81200*   -0.79800*

FILE:STLR50(22-03-79)
DATE:22-03-79 13.51

* PRL                                  Print results list
NR INTENSITY -------CONCENTRATION--------  APPARENT CONCENTR. IDENTIFICATION
          CHEMICAL CALCULATED    DIFF.   CHEMICAL CALCULATED
 1   0.370   0.42000   0.42014  0.00014   0.42880   0.42895 SS-61
 2   0.369   0.44000   0.42864 -0.01136   0.43970   0.42834 SS-62
 3   0.389   0.45000   0.44433 -0.00567   0.45907   0.45329 SS-63
 4   0.391   0.45000   0.45288  0.00288   0.45366   0.45656 SS-64
 5   0.567   0.67000   0.67086  0.00086   0.68459   0.68546 SS-65
 6   0.450   0.51000   0.51917  0.00917   0.52384   0.53326 SS-66
 7   0.439   0.50000   0.50782  0.00782   0.51140   0.51940 SS-67
 8   1.160   1.42000   1.41563 -0.00437   1.46199   1.45749 SS-68

* SRR 50                              Calculated values are acceptable, store constants in CP50 list
NEW LIST
NAME =                                    := STAINLESS STEELS  Identification of CP list
NDEC=    3 := 2   Number of decimals in concentrations readout
```

Note that the CP list identification is not requested in the following SRR dialogs.

```
* NRE                                  Next regression element
REGR. ELMNT := TI                     Regression analysis of Ti selected
```

Note that in this examples section the regression analysis is not shown for all elements.

```
* SRA
ELEMENT= TI        MODEL= DJ     SIGMA=    0.18271     K=    0.24712

      D             E       ALPHA(MO )  ALPHA(NB )  ALPHA(NI )  ALPHA(MN )
    0.01369      -0.00879      3.06500*    2.85600*    0.26500*   -0.11500*

 ALPHA(CR )  ALPHA(TI )  ALPHA(P2 )  ALPHA(S2 )  ALPHA(SI )
   -0.20000*    1.00500*    0.99000*    1.45600*    0.70000*

FILE:STLR50(22-03-79)
DATE:22-03-79 14.39

* PRL
NR INTENSITY -------CONCENTRATION--------  APPARENT CONCENTR. IDENTIFICATION
             CHEMICAL CALCULATED    DIFF.  CHEMICAL CALCULATED
 1    0.018  0.00000   0.01339   0.01339   0.00000   0.01353 SS-61
 2    0.017  0.00000   0.01370   0.01370   0.00000   0.01355 SS-62
 3    0.017  0.00000   0.01342   0.01342   0.00000   0.01354 SS-63
 4    0.021  0.46000   0.01366  -0.44634   0.45497   0.01351 SS-64
 5    1.346  0.00200   0.00185  -0.00015   0.00201   0.00186 SS-65
 6    0.037  0.00200   0.01428   0.01228   0.00187   0.01337 SS-66
 7    0.028  0.00000   0.01375   0.01375   0.00000   0.01344 SS-67
 8    0.024  0.00000   0.01344   0.01344   0.00000   0.01348 SS-68

* CCD 4 TI
   0.46000 := 0

* CCD 5 TI
   0.00200 := .46
```

Correction of a (deliberate) error in the concentration data, i.e. an input error during ACD.

```
* SRA
ELEMENT= TI        MODEL= DJ     SIGMA=    0.00207     K=    0.00652

      D             E       ALPHA(MO )  ALPHA(NB )  ALPHA(NI )  ALPHA(MN )
   -0.00787      0.34789      3.06500*    2.85600*    0.26500*   -0.11500*

 ALPHA(CR )  ALPHA(TI )  ALPHA(P2 )  ALPHA(S2 )  ALPHA(SI )
   -0.20000*    1.00500*    0.99000*    1.45600*    0.70000*

FILE:STLR50(22-03-79)
DATE:22-03-79 14.42

* PRL
NR INTENSITY -------CONCENTRATION--------  APPARENT CONCENTR. IDENTIFICATION
             CHEMICAL CALCULATED    DIFF.  CHEMICAL CALCULATED
 1    0.018  0.00000  -0.00152  -0.00152   0.00000  -0.00154 SS-61
 2    0.017  0.00000  -0.00212  -0.00212   0.00000  -0.00210 SS-62
 3    0.017  0.00000  -0.00188  -0.00188   0.00000  -0.00190 SS-63
 4    0.021  0.00000  -0.00052  -0.00052   0.00000  -0.00052 SS-64
 5    1.346  0.46000   0.45961  -0.00039   0.46089   0.46051 SS-65
 6    0.037  0.00200   0.00521   0.00321   0.00187   0.00488 SS-66
 7    0.028  0.00000   0.00208   0.00208   0.00000   0.00204 SS-67
 8    0.024  0.00000   0.00062   0.00062   0.00000   0.00062 SS-68

* SRR 50
NDEC=    3 := 2
```

Values acceptable and stored in CP50

```
* NRE                          Next regression analysis for Cr
REGR. ELMNT := CR

* SRA
ELEMENT= CR       MODEL= DJ     SIGMA=    0.72824     K=    0.17171

      D             E
   -5.36458      23.18992       Result not satisfactory

FILE:STLR50(22-03-79)
DATE:22-03-79 15.03

*CAL NI                         Attempt to obtain satisfactory result by calculating empirical alpha
                                value for nickel.

*SRA
ELEMENT= CR       MODEL= DJ     SIGMA=    0.60886     K=    0.14652

      D             E       ALPHA(NI )
   -3.28391      19.93202      0.64369   Result still not satisfactory

FILE:STLR50(22-03-79)
DATE:22-03-79 15.04

*RCF                            Reset of CAL N1

*CAL CR                         Attempt to get satisfactory result calculating empirical alpha value for chromium

*SRA
*** NO CONVERGENCE              Mathematical convergence not possible—empirical alphas do not produce
FILE:STLR50(22-03-79)           satisfactory results in this instance.
DATE:22-03-79 15.04

* FAL SI 1.226
* FAL P2 1.613
* FAL S2 2.23
* FAL TI 5.929                  Input of theoretical alphas
* FAL CR 1.495
* FAL MN .59
* FAL NI .77
* FAL NB 3.932
```

```
* SRA                    Regression of Cr, using theoretical alphas
ELEMENT= CR        MODEL= DJ      SIGMA=    0.11104      K=    0.02510

      D              E        ALPHA(MO )  ALPHA(NB )  ALPHA(NI )  ALPHA(MN )
    0.31563      12.48714       4.22700*    3.93200*    0.77000*    0.59000*

 ALPHA(CR )  ALPHA(TI )  ALPHA(P2 )  ALPHA(S2 )  ALPHA(SI )
    1.49500*    5.92900*    1.61300*    2.23000*    1.22600*

FILE:STLR50(22-03-79)
DATE:22-03-79 15.06

* PRL
NR INTENSITY -------CONCENTRATION--------  APPARENT CONCENTR. IDENTIFICATION
             CHEMICAL CALCULATED   DIFF.   CHEMICAL CALCULATED
 1   0.923   15.20000  15.23826  0.03826   11.81437  11.84410 SS-61
 2   0.769   12.80000  12.89799  0.09799    9.84635   9.92173 SS-62
 3   1.068   18.70000  18.63349 -0.06651   13.70531  13.65656 SS-63
 4   1.304   25.60000  25.77364  0.17364   16.48265  16.59445 SS-64
 5   1.033   18.45000  18.39801 -0.05199   13.25308  13.21573 SS-65
 6   0.943   17.60000  17.54050 -0.05950   12.12912  12.08811 SS-66
 7   0.999   17.80000  17.81247  0.01247   12.77656  12.78551 SS-67
 8   1.044   18.55000  18.40187 -0.14813   13.45755  13.35008 SS-68

* SRR 50                 Result is now satisfactory, and constants are saved.
NDEC=    3 :=  2
```

The regression analysis procedure is performed for all elements which will require an output showing apparent contcentration, or chemical concentration when unknown samples are measured. Apparent concentrations are calculated using the D and E constants, and chemical concentrations will additionally require alpha (and/or beta) constants to correct for interelement effects.

For each satisfactory element regression analysis the SRR command should be given to store the constants in the CP list.

The databank containing the regression results must be transferred to the disc containing the routine measurement results. Now replace the UP system disc by the AN disc, start the system, and then load the databank into the memory.

```
DATE :23 03 79
TIME :15 16                 Follow the procedure in paragraph 2.1.2.
X14-AN-00.0

* LDB 1400:1                Load databank to the memory

*
```

After the regression analysis of all elements, and transfer of the constants to the CP list (by SRR), the stored constants can be readout.

```
*FCF 50                                        Print calculation parameters.
 END OF REGRESSION=YE :=
CPNR= 50   STAINLESS STEELS                          MODEL=  DJ
```

ELM	ND	NC	D	E	CEL	ALPHA	CEL	ALPHA
SI	2	9	-0.05217	1.30101	MO	-0.34900	NB	-0.39300
					NI	0.26500	MN	-0.11600
					CR	-0.21400	TI	-0.64300
					P2	-0.84500	S2	-0.81200
					SI	-0.79800		
MN	2	9	-0.11009	0.60848	MO	1.55900	NB	1.41200
					NI	-0.11400	MN	0.32900
					CR	0.18900	TI	2.36300
					P2	0.26600	S2	0.56500
					SI	0.07500		
S2	3	9	0.00602	0.00809	MO	-0.13400	NB	-0.19100
					NI	0.26500	MN	-0.11300
					CR	-0.21600	TI	-0.54700
					P2	1.02600	S2	-0.61200
					SI	0.75100		
P2	3	9	0.00691	0.01408	MO	-0.29200	NB	-0.33800
					NI	0.26600	MN	-0.11600
					CR	-0.21400	TI	-0.60500
					P2	-0.72600	S2	-0.78700
					SI	0.76400		
NI	2	9	-0.15610	10.50491	MO	-0.54600	NB	-0.58400
					NI	-0.63700	MN	-0.09400
					CR	-0.18300	TI	-0.34900
					P2	-0.75600	S2	-0.69800
					SI	-0.79300		
CR	2	9	0.31563	12.48714	MO	4.22700	NB	3.93200
					NI	0.77000	MN	0.59000
					CR	1.49500	TI	5.92900
					P2	1.61300	S2	2.23000
					SI	1.22600		
MO	2	9	-0.00061	0.43359	MO	0.12000	NB	0.06600
					NI	0.21500	MN	-0.09200
					CR	-0.18800	TI	-0.35200
					P2	-0.76100	S2	-0.70300
					SI	-0.80100		
NB	2	9	-0.12330	0.77359	MO	-0.10900	NB	0.03800
					NI	0.21500	MN	-0.09300
					CR	-0.18800	TI	-0.35200
					P2	-0.76200	S2	-0.70200
					SI	-0.80100		
TI	2	9	-0.00787	0.34789	MO	3.06500	NB	2.85600
					NI	0.26500	MN	-0.11500
					CR	-0.20000	TI	1.00500
					P2	0.99000	S2	1.45600
					SI	0.70000		

```
* LDM 1
```

Load monitor sample

```
* SMM 50
```

Remeasure the monitor to update the stored intensities, and the readout also shows the percentage change compared with the previous measurement (mainly due to counting statistical spread)

```
*
  MP 50  CP 50  NET INTENSITIES                          22-03-79 15.24

      MO          NB          NI          MN          CR          TI          P2
    3036.       5197.      26831.       1054.      31073.      19343.        36.
     1.02%      -0.40%      -0.03%       1.71%      -0.16%       0.19%      3.35%

      S2          SI
      32.       2267.
    -4.01%       0.06%

* ULM 1

* SMX 50                                  Start measurement of unknown sample
SAM.POS= 1 I
IDENT 1= STAINLESS 25                    Loading and identification

*
  MP 50  CP 50  STAINLESS STEELS                         22-03-79 15.39
CONCENTRATIONS     STAINLESS 25

      SI          MN          S           P          NI          CR          MO
    0.60        1.88       0.018       0.027       11.99       17.41        2.42

      NB          TI
    0.01        0.02

* SMX 50                                  Measurement of a second sample
SAM.POS= 1 I
IDENT 1= STAINLESS 15

* PIN
```

Command given (before result readout commences) to also print a gross intensities readout

```
*
  MP 50  CP 50  STAINLESS STEELS                         22-03-79 15.46
GROSS INTENSITIES  STAINLESS 15

      MO          MO+         NB          NI          MN          CR          TI
    1327.        810.        848.      25878.      3145.       33026.       453.
     0.87%       2.48%       1.09%       0.14%       0.56%       0.12%      2.35%

      P2          P2+         S2-         S2          SI
      98.         32.         32.         72.       1052.
    1.60%       3.96%       3.93%       1.87%       0.69%

CONCENTRATIONS     STAINLESS 15

      SI          MN          S           P          NI          CR          MO
    0.54        1.76       0.015       0.032        9.00       18.59        0.07

      NB          TI
    0.00        0.00
```

Manual recalibration procedure (also refer to chapter 2.6.3.).

```
* WDD STL,1
```
Write data to disc in station 1, with identification STL

```
* SMR 50
RECALIBRATION FILE : STLB50,1
```
Start manual recalibration.
Note file type identification B50.

```
NR OF SAMPLES := 5
SAM.POS= 1 2 3 4 I
IDENT OF S  1 = SS-64
IDENT OF S  2 = SS-65
IDENT OF S  3 = SS-66
IDENT OF S  4 = SS-67
```
Total of 5 recalibration standards to be used.

First 4 samples are loaded and identified and measurement commences

```
* NPI
```
No gross intensity output required

```
*
  MP 50  CP 50  STAINLESS STEELS                          22-03-1979 16.13
INTENSITIES        SS-64

      MO          NB          NI          MN          CR          TI          P2
   0.02929     0.15621     2.43793     1.63029     1.30457     0.01908     0.47548

      S2          SI
   2.21490     0.38065

DATA TO FILE STLB50,1

INTENSITIES        SS-65

      MO          NB          NI          MN          CR          TI          P2
   0.07158     0.16712     1.01651     1.63418     1.03230     1.34622     0.82436

      S2          SI
   2.41175     0.56822

DATA TO FILE STLB50,1

INTENSITIES        SS-66

      MO          NB          NI          MN          CR          TI          P2
   5.62977     0.16806     1.03168     1.39384     0.94616     0.03637     1.02588

      S2          SI
   2.33663     0.45408

DATA TO FILE STLB50,1

INTENSITIES        SS-67

      MO          NB          NI          MN          CR          TI          P2
   0.09454     1.50030     1.01458     1.56845     0.99958     0.02876     0.68609

      S2          SI
   1.35610     0.43243

DATA TO FILE STLB50,1
```
First 4 recalibration standards have been measured and results are stored in the recalibration file on disc.

```
IDENT OF S  5 = SS-68
```

Fifth (and last) recalibration standard loaded and identified, and measurement commences.

```
*
  MP 50  CP 50  STAINLESS STEELS
INTENSITIES          SS-68                    22-03-1979 16.21

      MO          NB          NI          MN          CR          TI          P2
 0.06951     0.15934     1.00619     2.66951     1.04417     0.02518     1.11366

      S2          SI
 2.49542     1.15468

DATA TO FILE STLB50,1
```

Fifth standard measured and results stored on disc.

```
RECALIBRATION OF MO
D = YE :=
E = YE :=
USE ALL SAMPLES = YE :=
APPARENT CONCENTRATIONS:
```

Recalibration input for first element in MP-list.
Recalibration of both slope and intercept required.

All samples to be used for the recalibration

```
S 1 := .0179
S 2 := .03493
S 3 := 2.46656
S 4 := .03473
S 5 := .03751
```

Input of apparent concentrations

```
ELM   S1 S2      D(NEW)      D(OLD)      E(NEW)      E(OLD)
MO     0  0     0.00238    -0.00061     0.43749     0.43359   SAVE=YE :=
```

Recalibration results are acceptable and are saved to update the CP-list.

```
RECALIBRATION OF NB
D = YE :=
E = YE :=
USE ALL SAMPLES = YE :=
APPARENT CONCENTRATIONS:
```

Next element, and so on

```
S 1 := -.00313
S 2 := .00527
S 3 := .00523
S 4 := 1.03785
S 5 := .00158
ELM   S1 S2      D(NEW)      D(OLD)      E(NEW)      E(OLD)
NB     0  0    -0.12369    -0.12330     0.77414     0.77359   SAVE=YE :=

RECALIBRATION OF NI
D = YE :=
E = YE :=
USE ALL SAMPLES = YE :=
S 1 := 25.40969
S 2 := 10.53249
S 3 := 10.66006
S 4 := 10.46544
S 5 := 10.44632
ELM   S1 S2      D(NEW)      D(OLD)      E(NEW)      E(OLD)
NI     0  0    -0.12984    -0.15610    10.47550    10.50491   SAVE=YE :=
```

```
RECALIBRATION OF MN
D = YE :=
E = YE :=
USE ALL SAMPLES = YE :=
APPARENT CONCENTRATIONS:
S 1 :=  .90954
S 2 :=  .91647
S 3 :=  .74736
S 4 :=  .85413
S 5 := 1.53420
ELM   S1 S2      D(NEW)      D(OLD)      E(NEW)      E(OLD)
MN     0  0    -0.10007    -0.11009     0.61392     0.60848   SAVE=YE :=
RECALIBRATION OF CR
D = YE :=
E = YE :=
USE ALL SAMPLES = YE :=
APPARENT CONCENTRATIONS:
S 1 := 16.59445
S 2 := 13.21573
S 3 := 12.08811
S 4 := 12.78551
S 5 := 13.35008
ELM   S1 S2      D(NEW)      D(OLD)      E(NEW)      E(OLD)
CR     0  0     0.25362     0.31563    12.53395    12.48714   SAVE=YE :=
RECALIBRATION OF TI
D = YE := -.00052          Input error, question is repeated.
D = YE :=
E = YE :=
USE ALL SAMPLES = YE :=
APPARENT CONCENTRATIONS:
S 1 := -.00052
S 2 :=  .46051
S 3 :=  .00488
S 4 :=  .00204
S 5 :=  .00062
ELM   S1 S2      D(NEW)      D(OLD)      E(NEW)      E(OLD)
TI     0  0    -0.00775    -0.00787     0.34782     0.34789   SAVE=YE :=

RECALIBRATION OF P2
D = YE :=
E = YE :=
USE ALL SAMPLES = YE :=
APPARENT CONCENTRATIONS:
S 1 :=  .01333
S 2 :=  .0185
S 3 :=  .02402
S 4 :=  .01551
S 5 :=  .02237
```

```
ELM   S1 S2      D(NEW)      D(OLD)      E(NEW)      E(OLD)
P2     0  0     0.00492     0.00691     0.01674     0.01408   SAVE=YE :=

RECALIBRATION OF S2
D = YE := .02248
D = YE :=
E = YE :=
USE ALL SAMPLES = YE :=
APPARENT CONCENTRATIONS:
S 1 := .02248
S 2 := .02469
S 3 := .02427
S 4 := .01739
S 5 := .02526
ELM   S1 S2      D(NEW)      D(OLD)      E(NEW)      E(OLD)
S2     0  0     0.00795     0.00602     0.00687     0.00809   SAVE=YE :=

RECALIBRATION OF SI
D = YE :=
E = YE :=
USE ALL SAMPLES = YE :=
APPARENT CONCENTRATIONS:
S 1 :=.45656
S 2 := .68546
S 3 := .53326
S 4 := .5194
S 5 := 1.45749
ELM   S1 S2      D(NEW)      D(OLD)      E(NEW)      E(OLD)
SI     0  0    -0.04568    -0.05217     1.29770     1.30101   SAVE=YE :=

*
```

Input error, question is repeated

Last element

Recalibration procedure is now complete resulting in an updated CP-list and a recalibration file STLB50 on the disc in station 1.

Automatic recalibration procedure. The semiautomatic recalibration is not shown here: refer to chapter 2.6.4. The semiautomatic recalibration procedure is identical to the automatic one except for the last part where one can accept or refuse the recalibration data.

```
*^WDD STL,1
```
Write data to disc, file STL

```
*\SAR 50
```
To get access to recalibration file STLB50

```
RECALIBRATION FILE : STLB50,1
GIVE CR AFTER LOADING S  1 : SS-64
GIVE CR AFTER LOADING S  2 : SS-65
GIVE CR AFTER LOADING S  3 : SS-66
GIVE CR AFTER LOADING S  4 : SS-67
```
Recalibration standards are loaded as requested. Then measurement commences for first 4 standards, as specified during SMR.

```
*
  MP 50  CP 50  STAINLESS STEELS                    22-03-1979 17.35
INTENSITIES        SS-64

      MO          NB          NI          MN          CR          TI          P2
   0.03713     0.15186     2.43781     1.63760     1.30508     0.01914     0.53168

      S2          SI
   2.17231     0.38517

DATA TO FILE STLB50,1

INTENSITIES        SS-65

      MO          NB          NI          MN          CR          TI          P2
   0.08512     0.16119     1.01521     1.64186     1.03250     1.34211     0.84048

      S2          SI
   2.56681     0.57001

DATA TO FILE STLB50,1

INTENSITIES        SS-66

      MO          NB          NI          MN          CR          TI          P2
   5.61168     0.16275     1.03176     1.40428     0.94602     0.03659     0.96691

      S2          SI
   2.23033     0.45455

DATA TO FILE STLB50,1

INTENSITIES        SS-67

      MO          NB          NI          MN          CR          TI          P2
   0.08756     1.50282     1.01202     1.53365     0.99970     0.02908     0.53872

      S2          SI
   1.46196     0.43186

DATA TO FILE STLB50,1
```
Measurement on first 4 samples finished.

```
GIVE CR AFTER LOADING S  5 : SS-68
```

Loading of 5th standard and measurement commences.

```
*
  MP 50  CP 50  STAINLESS STEELS                          22-03-1979 17.41
INTENSITIES        SS-68

      MO          NB          NI          MN          CR          TI          P2
   0.08654     0.15623     1.00600     2.64371     1.04541     0.02441     1.0010

      S2          SI
   2.49607     1.15419

DATA TO FILE STLB50,1
```

Measurement on last sample finished.

ELM	S1	S2	D(NEW)	D(OLD)	E(NEW)	E(OLD)
MO	0	0	-0.00120	0.00259	0.43966	0.43996
NB	0	0	-0.11945	-0.12385	0.77009	0.77983
NI	0	0	-0.11274	-0.11330	10.46895	10.46955
MN	0	0	-0.11873	-0.10643	0.62689	0.61735
CR	0	0	0.26810	0.08134	12.51584	12.69978
TI	0	0	-0.00777	-0.00767	0.34889	0.34721
P2	0	0	0.00418	0.00385	0.01877	0.01902
S2	0	0	0.00721	0.00866	0.00714	0.00635
SI	0	0	-0.05001	-0.05183	1.30247	1.31046

Recalibration data are calculated according to the procedure and using the apparent concentrations as specified during SMR.

```
*
```

The resultant update of the calibration line as present in the D and E values in the CP-list can be shown using PCP.

* PCP 50
CPNR= 50 STAINLESS STEELS MODEL= DJ

ELM	ND	NC	D	E	CEL	ALPHA	CEL	ALPHA
SI	2	9	-0.05001	1.30247	MO	-0.34900	NB	-0.39300
					NI	0.26500	MN	-0.11600
					CR	-0.21400	TI	-0.64300
					P2	-0.84500	S2	-0.81200
					SI	-0.79800		
MN	2	9	-0.11873	0.62689	MO	1.55900	NB	1.41200
					NI	-0.11400	MN	0.32900
					CR	0.18900	TI	2.36300
					P2	0.26600	S2	0.56500
					SI	0.07500		
S2	3	9	0.00721	0.00714	MO	-0.13400	NB	-0.19100
					NI	0.26500	MN	-0.11300
					CR	-0.21600	TI	-0.54700
					P2	1.02600	S2	-0.61200
					SI	0.75100		
P2	3	9	0.00418	0.01877	MO	-0.29200	NB	-0.33800
					NI	0.26600	MN	-0.11600
					CR	-0.21400	TI	-0.60500
					P2	-0.72600	S2	-0.78700
					SI	0.76400		
NI	2	9	-0.11274	10.46895	MO	-0.54600	NB	-0.58400
					NI	-0.63700	MN	-0.09400
					CR	-0.18300	TI	-0.34900
					P2	-0.75600	S2	-0.69800
					SI	-0.79300		
CR	2	9	0.26810	12.51584	MO	4.22700	NB	3.93200
					NI	0.77000	MN	0.59000
					CR	1.49500	TI	5.92900
					P2	1.61300	S2	2.23000
					SI	1.22600		
MO	2	9	-0.00120	0.43966	MO	0.12000	NB	0.06600
					NI	0.21500	MN	-0.09200
					CR	-0.18800	TI	-0.35200
					P2	-0.76100	S2	-0.70300
					SI	-0.80100		
NB	2	9	-0.11945	0.77009	MO	-0.10900	NB	0.03800
					NI	0.21500	MN	-0.09300
					CR	-0.18800	TI	-0.35200
					P2	-0.76200	S2	-0.70200
					SI	-0.80100		
TI	2	9	-0.00777	0.34889	MO	3.06500	NB	2.85600
					NI	0.26500	MN	-0.11500
					CR	-0.20000	TI	1.00500
					P2	0.99000	S2	1.45600
					SI	0.70000		

2.8.3. Databank and parameterbank operation

In this paragraph the databank and parameterbank operation related to the examples given in 2.8.1. and 2.8.2. is shown.

Starting from initial start-up and the situation that nothing has yet been assembled in the databank and parameterbank, PMM and PPB read out as follows:

```
.R PW1400                          Initiation

X14D-002.0

* PMM                              Print memory map, databank contents. Note that databank
SY0:PW1400                         PW 1400 is automatically loaded from the disc in station 0.(SY0)
LP   0
FREE SPACE   2986 WORDS            Empty databank (computer memory and disc).

* PPB                              Print parameter bank contents.

FREE SPACE :   848 WORDS           Empty parameter bank (microprocessor).

*
```

Now, before assembly commands are input, the empty databank is copied onto the disc in station 1 and in this case the name "DB1400" is chosen.

```
* WDB DX1:DB1400                   Write databank to disc in station 1; identification DB1400.
```

This (empty) databank is then loaded into the computer memory

```
* LDB DX1:DB1400                   Load databank from disc in station 1, identification DB1400.

* PMM
DX1:DB1400                         Now databank DB1400 is in memory
LP   0
FREE SPACE   2986 WORDS            Still empty
```

Now assembly input is given which is stored in the databank (computer memory and on disc) from commands like ALP, ACP, ARC, AML, AMS, ANM, AMB, ALL.
Also, assembly input is given which is stored in the parameter bank (microprocessor) from commands like ACH, AMP and AJB.
After this assembly input, PMM and PPB read out as follows:

```
* PMM
DX1:DB1400
LP  0 10 50
ML 10
MS  1  2  3  4  5
CP 10 50
MB 50
LL 50
RC  1  2
FREE SPACE  2438 WORDS
```

Information in databank

A detailed readout can be obtained from PLP, PMB, PCP, PML, PMS, PLL, PRC, etc.

```
* PPB
F   F2  NA  MG  MG2 AL  SI  P   P2  S   S2  CL  K   CA  CA2
TI  V   CR  MN  FE  CO  NI  CU  CU2 ZN  GA  GE  AS  SE  BR
RB  SR  Y   ZR  NB  MO  RU  RH  PD  AG  CD  IN  SN  SB  TE
I   CS  BA  LA  CE  HF  TA  W   RE  OS  IR  PT  AU  HG  PB
BI  RA  U

MP 10
MP 50
FREE SPACE :  796 WORDS
```

Information in parameter bank

A detailed readout can be obtained from PCH and PMP.

The information in the databank is also present in the databankfile on disc (recorded automatically during assembly). A record on disc of the information in the parameter bank is made using DPB. The same disc station and file name as the loaded databank are used to record the parameter bank.

```
* DPB
DATA TO FILE DX1:DB1400

*
```

Dump parameter bank data to disc.

Disc station and file name same as databank,

On the disc in station 1, two files exist now: a databank file and a parameter bank file which have the same name, but can be distinguished by the file type identification which is added automatically by the system.

```
* END                                    End X14D software

.DIR DX1:                               Print directory of disc in station 1.
 29-Oct-79
DB1400.DBK      5 29-Oct-79        DB1400.PBK      3 29-Oct-79
 2 Files, 8 Blocks
 472 Free blocks

.R PM1400

X14D-002.0


*
```

Each time the computer is switched off, the databank has to be read-in again using LDB DX1 : DB 1400.
Note that the information in the parameter bank is neither affected by computer switch-off nor spectrometer switch-off (refer to 1.3.4.), nor loading of other databanks.
The parameter bank information can be read in from the file on disc into the microprocessor by RPB (after loading the appropriate databank).

```
* CPB                                    Clear parameter bank

* PPB                                    Empty parameter bank readout to show the effect of CPB.

FREE SPACE :  848 WORDS

* LDB DX1:DB 1400                        Load appropriate databank

* RPB                                    Read the corresponding parameter bank from disc into the microprocessor.

* PPB                                    Parameter bank data present in microprocessor memory again.
F    F2   NA   MG   MG2  AL   SI   P    P2   S    S2   CL   K    CA   CA2
TI   V    CR   MN   FE   CO   NI   CU   CU2  ZN   GA   GE   AS   SE   BR
RB   SR   Y    ZR   NB   MO   RU   RH   PD   AG   CD   IN   SN   SB   TE
I    CS   BA   LA   CE   HF   TA   W    RE   OS   IR   PT   AU   HG   PB
BI   RA   U

MP 10
MP 50
FREE SPACE :  796 WORDS

*
```

CHEMICAL CONCENTRATION	As manually input (ACD command).
CALCULATED CONCENTRATION	Based on the intensity values and using the available D, E, α and β values, in the selected calculation model.
CONCENTRATION DIFFERENCE	The difference between the chemical and calculated values.
CHEMICAL APPARENT CONCENTRATION	Equal to chemical/1 + Δ, where Δ represents the matrix correction, e.g. $\Sigma \alpha$ C for the DJ model.
CALCULATED APPARENT CONCENTRATION	Equal to $C_A = (D + ER)$
IDENTIFICATION	Identification of the standard samples, as input after the SPR command.

When the regression results are satisfactory they can be automatically transferred to the CP list by giving **SRR** (save regression results). The regression routine then continues for the next element by giving **NRE** (next regression element).

If a graphical terminal is connected the regression results can be plotted with **PLT**, which aids evaluation of the results.

10.4.1. Prepare for regression analysis

The regression analysis calculation routine requires intensity and concentration values for each element in the set of standard samples. These data are stored in a file on the files disc in disc drive 1.

When the calibration standard samples are ready for analysis, the system disc AN must be in station 0, and the files disc in disc drive 1. Give a write data to disc command WDD xxx, where xxx is a three character identification relating to the type of samples to be analysed, e.g. STE for steels as the example in figure 10.4A.

Now give the SPR (start prepare regression) command, and define the measurement program to be used. This number will be incorporated in the file type identification.

The dialog requests sample identification to be typed, and the standard samples are loaded and measured. The readout shows the intensity values which have been written to the files disc. Repeat the procedure by typing c.r. only followed by typing the sample identification until all samples have been measured, then give NDD (no data to disc) to prevent any undesired writing of data in future.

Type END, remove the AN system disc and replace with the UP (update) system disc, (files discs still in station 1), and initiate the system — switch to mid-position, operate INST, MC and IPL (mini-panel operate START), input date and time or give c.r.'s, and then switch to LOCK.

The regression intensities file on the files disc must now be opened by giving the OPF command, where the same identification is given as printed after the "DATA TO FILE ---" output, figure 10.4A.

Now give the ACD (add concentration data) command to add the known chemical concentration values of the standard samples to the file in the files disc, see figure 10.4B. The dialog will request an input of concentration values for **all** elements in all the standard samples which have been measured, so type the known value or give a carriage return (or zero). Carriage return only will be interpreted as zero.

3. OPTIONAL ACCESSORIES

This paragraph describpes the operation of the various accessories which can be supplied with the PW1400 Spectrometer system. These options are:

PW 1500/00	6 position sample loader
PW 1500/10	72 position sample changer
PW 1464/50	Helium flushing system
PC 1409/00	Teleprinter
P817-001	Video display terminal
Graphical terminal	

3.1. PW 1500/00 6 POSITION SAMPLE LOADER

The sample loader can be fitted to the front of the spectrometer so that a tray of up to six samples can be automatically loaded into the spectrometer for measurement. An addition which can be supplied with the PW 1500/00 is the PW 1505/00 Reference tray option, which allows reference, re-calibration or other samples to be stored outside the sample turret.

3.1.1. Operation

The following commands can be used when a PW 1500/00 sample loader is installed:

LTU i	Load sample from the changer into turret position i, where i = 1 to 4.
UTU i	Unload sample from turret position i to the changer, where i = 1 to 4.
ASC i (j)	Automatic sample changer to be used for the measurement of samples in tray i, where i = 1 to 165. The optional argument is an identification number from 0 to 999, which is raised by 1 for each new sample loading.
SMX	Start measurement of unknown samples using the sample loader.
PTY i	Programmed tray i, where i = 1 to 165, can have a separate measurement program and sample identification for each sample.
RES	Reset the recycle and ASC commands.

In addition the following commands are used when a PW 1505/00 Reference tray option is fitted:

FRT	Fetch the reference tray to load the sample from position 1 to the spectrometer.
SRT	Store the sample tray from the loader to the reference tray position (PW 1505).

A list of stop commands and error messages is given in paragraph 3.2.1.

Identification card

A blank identification card is shown in paragraph 3.2.2. and a quantity will be supplied (50 per PW 1501 set of 5 trays). The card must define the measurement program list number for automatic operation, the tray identification number, and M bit for monitor measurement.

Sample loading

A tray of up to six samples can be loaded into the left-hand position of the sample loader, so that the identification card on the front of the tray is in front of the card reader. A further tray of samples can be prepared for analysis, if required, during the measurement of the samples in the tray in the loader.

Reference tray option

A tray of reference or recalibration samples can be stored in the PW 1505/00, if fitted, and when these samples are to be measured the reference tray will be transported to the loading position of the PW 1500/00 when the FRT command is given. The SRT command should be given after the samples have been measured and reloaded in the tray, in order to return the reference tray to the PW 1505 option. Note that FRT and SRT can be assembled in a job list for automatic execution of loading, measurement and unloading.

Sample measurement

A tray of samples can be measured automatically (identification card control) using the ASC command, manually by using separate keyboard commands, or by using an assembled job list.

Keyboard controlled measurement is only possible if a previous ASC command is cancelled by RES. The loader and spectrometer operation is controlled from the keyboard, such as position the tray (MTY i), load/unload samples (LTU i/UTU i), and sample measurement (SMX i, i, or c.r.).

When the ASC command is given, and other instrument conditions set (SPN, CMD, RCS, etc.) , the start measurement command will initiate the automatic measurement of all samples in the tray, and samples will be returned to their original positions after results readout. The start measurement command can be SMX (no program number assignment) or a carriage return, or SPR, SMA, SMR, SSR or SAR.

Note that when the ASC command is given the argument i is necessary, which will normally be the tray number punched out on the identification card. In this case the samples in the tray are measured, returned to the tray, and the tray is moved to the right-hand position in the loader and the sample measurement stops. If the i argument is not equal to the identification card number an error message will be output.

The comments shown later for the PW 1500/10 regarding monitor measurement, batch/continuous mode, job measurement, etc., will generally apply to the sample loader operation. Note that a job measurement can be assembled to include commands such as FRT, MTY, LTU i, SMX i, UTU i, etc. and SRT.

A job list can be prepared to handle various functions, for example to measure a tray, fetch the reference tray (FRT), load and measure the monitor samples to update stored monitor results (PW 1505 fitted), unload the samples and store the reference tray again. The reference tray samples can only be measured in the keyboard controlled mode or by SJB using a job list.

NOTE: **Note that SJB and SMM cannot be given in the ASC mode, in which case the error message ERROR SAMPLE CHANGER CODE 00 is generated. If necessary reset ASC by typing RES after which SJB and SMM are allowed.**

3.1.2. Description (PW 1500/00 and PW 1505/00)

The sample loader can be bolted to the front of the spectrometer, and it comprises a tray movement mechanism, a grab arm mechanism, and the necessary control circuits. The main control circuit is fitted in the right-hand side of the spectrometer, and a sample holder light-beam detector is mounted at the sample loading hole.

The reference tray option (PW 1505/00) can be supplied with, or added to, the sample loader. It comprises a tray storage position and a load/unload tray mechanism. Apart from a small drive circuit board, the necessary control electronics are provided in the basic sample loader. This option will require connection to the compressed air supply in the PW 1400.

3.2. PW 1500/10 72 POSITION SAMPLE CHANGER

The sample changer can be attached to the front of the spectrometer to allow the automatic (or manual) analysis of samples. These samples are loaded into six-position sample trays, and up to 12 trays can be loaded into the changer.

3.2.1. Commands and error messages

The following commands can be used when a PW 1500/10 Sample changer is installed:

STY i	Search for tray number i, where i = 1 to 165 (coded on the identification card). The changer will search until position 1 of the selected tray number i is in position ready to be loaded into the spectrometer.
MTY i	Move the tray to bring the tray position i ready for loading, where i = 1 to 6.
LTU i	Load sample from the changer into turret position i, where i = 1 to 4.
UTU i	Unload sample from turret position i to the changer, where i = 1 to 4.
ASC i (j)	Automatic sample changer to be used for the measurement of samples up to, and including, tray i, where i = 1 to 165. The optional argument j is an identification number from 0 to 999, which is raised by 1 for each new sample loading.
SMX	Start measurement of unknown samples using the sample changer.
RCS i	Recycle sample changer measurements i times, where i = 0 to 127, and 0 means infinity.
PTY i	Programmed tray i, where i = 1 to 165, can have a separate measurement program and sample identification for each sample.
RES	Reset the recycle and ASC commands.

Stop commands

/M	Stop after the completion of the measuring program of the samples. Used to interrupt a recycling program, or to interrupt a measurement routine using the automatic sample changer. The original recycling command is not reset.
/T	Stop after the complete measurement of samples in a tray in the loading position of the automatic sample changer. The next start measurement command will commence measurement of the samples in the next tray.
/	Stop measurement program (or other action) immediately after slash and carriage return given. Samples in the turret will be unloaded to the tray, and the tray goes to position 1 (rest position)
/c.r./c.r.	Stop measurement, and stop other actions. Reverts immediately to C = mode.
/S	Stop the scaler/timer operation and print the results, if a further measurement is programmed this will start after the printout of the results.
BREAK or INTERRUPT	Stop immediately, interrupt any action. This action is prefered to /c.r. For use with PW1790/10 minicomputer.

Error messages

In addition to the normal spectrometer error messages, an error message "** ERROR SAMPLE CHANGER, CODE xx" can be output.
The coding of these errors is as follows:

CODE	MEANING
00	SJB and SMM not allowed in ASC mode.
04	Mechanical drive faulty for tray movement at front side of changer
08	Similar error for tray movement at spectrometer side
20	Similar error for queueing (belt drive motor)
24*	PW 1505 Reference tray movement error (FRT/SRT)
10	Mechanical horizontal drive faulty to grab arm
40	Mechanical vertical drive faulty to grab arm
E0	Tray drive at front side (M2) not in the rest position
E1	No tray transport at front side (S16 operated)
F0	Sample changer not connected
F1	Cap not high (up), during UTU or LTU
F2	Sample already in spectrometer loading hole
F3	Sample not in spectrometer
F4*	FRT or SRT movement not possible
F5	Sample in tray
F6	Sample not in tray
F7	Grab arm in position at spectrometer, therefore, cap up/down is inhibited
F8	Tray drive at the spectrometer side (M1) not in the rest position
F9	Grab arm not in the rest position (not low)
FA	Tray not at the spectrometer side
FB	Tray movement inhibited – S13 operated
FC	Tray movement inhibited – S14 operated
FD*	Tray not in PW 1505 loader, or incorrect tray (FRT/SRT)
FE*	Reference option not in loader
FF	Optical reader error

* These errors only apply to the sample loader and/or reference tray option.

The figure below shows the general layout of the tray drive and position microswitches of the sample changer, which can be used to assist the rectification of simple faults.

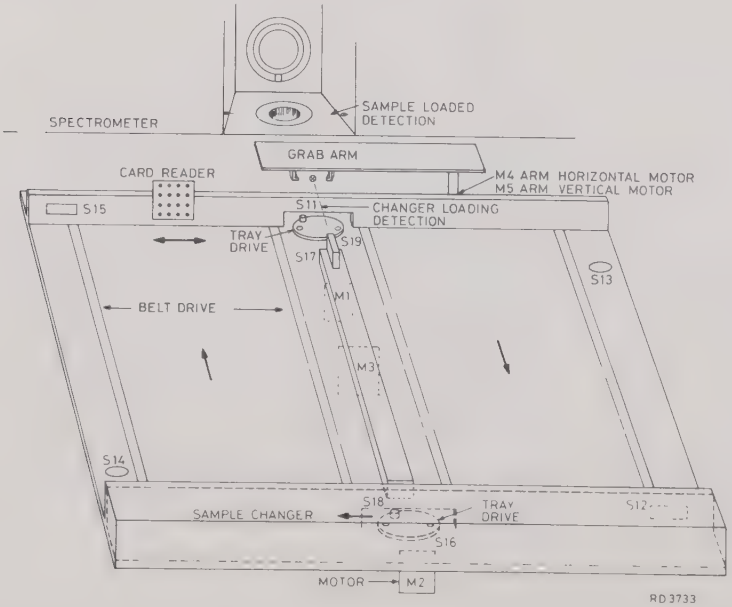
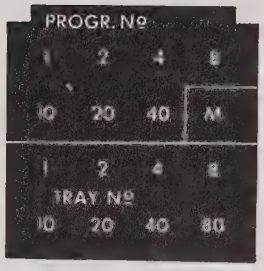


Fig. 3.2A. General layout of the sample changer

3.2.2. Identification card

NAME:

A blank identification card is shown, and a quantity of these will be supplied (50 per PW 1501). For automatic sample changing operation each tray must have an identification card inserted in the central side slots of the tray. Ensure that the cards are correctly located to ensure a proper output from the changer card reader.



Coding is set by pushing out the circular discs to allow identification by the card reader from the reflective surface.

The **program number** must be an **MP** (see paragraph 3.2.4.) or a job list (see paragraph 3.2.10.) which is stored in the parameter bank, otherwise an error message is generated.

The **M** disc is pushed out when it is desired to perform a ratio measurement (buffer or direct ratio). The monitor sample is either already in the turret, or is in the first position of the tray, see paragraph 3.2.4.

The **tray** number is used to identify a sample tray (between 1 and 165), and when the sample changer is loaded the operator should ensure that two trays should not have the same number. The tray number i given in the ASC i command indicates the last tray to be measured. The identification number (TRAY N°) will be printed in the results output, see paragraph 3.2.5.

3.2.3. Sample loading

Unknown, monitor and other samples are inserted into the normal sample holders, which can then be placed into the sample trays, Up to 6 samples can be placed in a tray, and up to 12 trays in a sample changer.
The weight of any sample must not exceed 400 grammes.
The trays can then be placed on the sample changer table, with the identification cards facing the spectrometer.

When the ASC command is used the sample changer will load samples, and unload them after measurement, automatically. The load/unload procedure will be determined by the selection of the mode of operation (BMD or CMD), and by the loading of monitor samples into the turret (LDM), refer to paragraph 3.2.7. Alternatively, monitor samples can be placed in position 1 of the sample tray(s).

When jobs are executed in the automatic (ASC) command, i.e. the card program number is not an MP list but is a job list, the sample will only be loaded in turret position 4.

Empty positions in the sample tray will be skipped, and samples will be returned to their original positions in the tray after measurement e.g. if positions 1 and 3 have samples loaded but position 2 is empty, position 2 will not be filled with a sample after measurement.

When samples are measured under keyboard control (ASC not input) the comments above regarding sample positioning are still valid, but loading and unloading operations are initiated by commands such as LTU, UTU, etc., refer to paragraph 3.2.11.

3.2.4. Sample measurement

The measurement of samples from the sample changer will normally be carried out automatically (ASC command), but keyboard controlled operation is possible.

- Automatic control.
  All (or part) of the trays loaded in the sample changer can be automatically measured when the ASC command is given. Other instrument conditions can be set, such as SPN, SOT, RCS, etc., before the measurement commences from SMX (no argument), or carriage return.

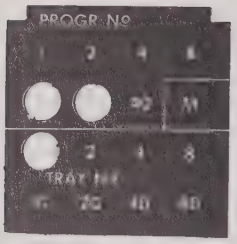
The operation of automatic sample changer measurement is illustrated by an example, using simple measurement programs, as follows:

Tray – card not inserted.
Tray 1 card shows an MP list which has not been assembled (also not a job list).
Tray 2 five samples measured in absolute mode.
Tray 3 two samples measured in direct ratio mode with monitor already loaded in turret position 1.
Tray 4 one monitor sample and two unknown samples in buffer ratio mode (using monitor turret position 2.)
Tray 5 as 4, but two samples and M bit not pushed out in ident. card.
Tray 6 a job measurement.

```
C=PPB

F    F2   NA   MG   MG2  AL   SI   P    P2   S    S2   CL   K    CA   CA2
TI   V    CR   MN   FE   CO   NI   CU   CU2  ZN   GA   GE   AS   SE   BR
RB   SR   Y    ZR   NB   MO   RU   RH   PD   AG   CD   IN   SN   SB   TE
I    CS   BA   LA   CE   HF   TA   W    RE   OS   IR   PT   AU   HG   PB
BI   RA   U

MP 31
MP 32
MP 33
JB 41
FREE SPACE :  818 WORDS
```

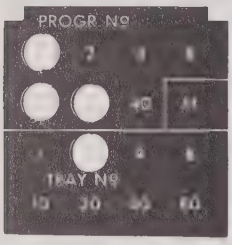
Tray 1 MP list not assembled

Trays 1-6



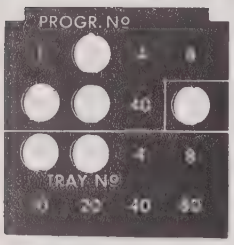
Tray 1 empty

Tray 2



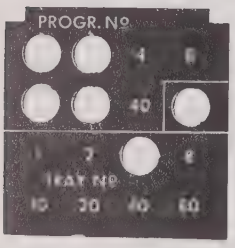
```
MP 31      for tray 2

MASK :  1
ABS  : YE     Absolute

CHAN    PT    PC
CU       2   0E0
```

Tray 3



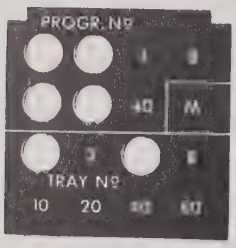
```
MP 32      for tray 3

MASK :  1
ABS  : NO  | Direct
BRAT : NO  | ratio
MOPS :  1  |
MOMPY:  1  |

CHAN    PT    PC
FE       2   1E5
```

Tray 4



```
MP 33      for tray 4 and 5

MASK :  1
ABS  : NO  | Buffer
BRAT : YE  | ratio
MOPS :  2
MOMPY:  1

CHAN    PT    PC
ZN       2   0E0
```

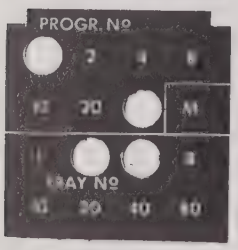
Tray 5



Job list for tray 6

```
C=AJB 41

J=SCH CU

J=SLF 44.5

J=PTS 1

J=STS 45.5 .1

J=EJB
```

Tray 6



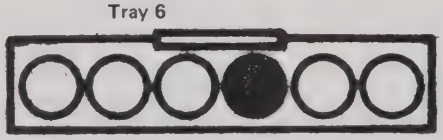


Fig. 3.2B Sample changer measurements (page 1 of 2)

```
C=BMD
```
Batch mode

```
C=LDM 1
```
Load monitor to turret position 1, for MP 32

```
C=ASC 6
```
Automatic sample changing until tray 6 is measured

```
C=SMX
```
Start measuring unknowns. Loading and measurement starts

```
TRAY    0     0
** NOT IN MEMORY
```
Empty tray read-out (card not fitted)

```
TRAY    1    30
** NOT IN MEMORY
```
Tray 1 with MP list 30, which is not assembled, therefore an error message printed, tray skipped

```
TRAY    2    31
```
Tray 2 (MP list 31) measurement starts on 5 samples

```
MP 31   3 SAMPLES     1 CHANNELS   MOPS   0
T  2 2 : 0021           3 : 0022           4 : 0024
CU       140278    2.000    143748    2.000    147220    2.000
```
First 3 samples loaded (turret position 1 is occupied by monitor). Note tray/position output. Results output

```
MP 31   2 SAMPLES     1 CHANNELS   MOPS   0
T  2 2 : 0025           3 : 0026
CU       123948    2.000    126614    2.000
```
Samples unloaded and next two samples loaded.

```
TRAY    3    32   M
```
Direct ratio mode measurement

```
MP 32   2 SAMPLES     1 CHANNELS   MOPS   1
T  3 1 : MONITOR        2 : 0031           3 : 0032
FE       100000    1.145    100000    1.823    100000    1.553
```
Two unknowns loaded and measured together with monitor in position 1. Two unknown samples unloaded.

```
TRAY    4    33   M
```
Buffer ratio, note M bit and monitor in position 1 of tray (monitor in turret not used).

```
MP 33   0 SAMPLES     1 CHANNELS   MOPS   2
T  4 2 : MONITOR
ZN      1045856    2.000
```
monitor loaded, measured and unloaded.

```
MP 33   2 SAMPLES     1 CHANNELS   MOPS   0
T  4 2 : 0042           3 : 0043
ZN       958896    2.000   1220377    2.000
```
Unknowns loaded, measured and unloaded.

```
TRAY    5    33
```
Buffer ratio (note M bit not pressed out, therefore no monitor measurement). Two unknown samples loaded.

```
MP 33   2 SAMPLES     1 CHANNELS   MOPS   0
T  5 2 : 0054           3 : 0055
ZN      1218379    2.000    958499    2.000
```
Measurement results. Samples unloaded.

```
TRAY    6    41
```
Job list 41 measurement

```
JB 41
 45.000          0      .000   CU
 44.500          0      .000
 44.500        471    1.000
 44.600       1004    1.000
 44.700       3211    1.000
 44.800      13496    1.000
 44.900      42071    1.000
 45.000      62991    1.000
 45.100      53562    1.000
 45.200      30953    1.000
 45.300      13203    1.000
 45.400       4594    1.000
 45.500       1606    1.000
C=
```
Set copper channel

Step scan results

Last tray ready, back to C = dialog

Fig. 3.2B. (page 2 of 2)

Figure 3.2B. shows the readout from the measurement of the samples in the above trays, and also shown are the print of the simple measurement programs used, and sketches of the tray/sample arrangements and the identification cards.

NOTE: **Note that SJB and SMM cannot be given in the ASC mode, in which case the error message ERROR SAMPLE CHANGER CODE 00 is generated. If necessary the ASC mode is reset by RES after which SJB and SMM are allowed.**

When the ASC command is given, SMX will start the measurement of the unknown samples. For regression measurements the SPR command must be given after ASC, and for recalibration procedures the SMR, SSR or SAR commands are used, refer to paragraphs 3.2.8. and 3.2.9.

Stop measurement.

Sample measurement will stop after any one of the following conditions:

1. The last tray (identification number = i) samples have been measured and returned to the tray.
2. A stop command is given (e.g. /c.r.)
3. An error condition is detected.

Note that /c.r./c.r. can be given to stop any changer or spectrometer movement.

3.2.5. Sample identification

The output of measurement results will firstly show "TRAY", the tray number, the program number and M if the M bit is pushed out, as given by the tray identification card. The readout of measurement results for each sample will show an identification composed of four digits, where the first three show the tray number, and the final digit shows the sample position in the tray. If the second (optional) argument j is given in the ASC command, this identification number (0 to 999) will be printed in place of the four digits for the first sample measurement result. The identification number is raised to one for each successive sample measurement result readout until the ASC command is reset.

3.2.6. Batch/continuous mode

Sample analysis using the changer can be performed in the batch or continuous mode by giving the command BMD or CMD before measurement commences, and this will determine the order of loading samples into the turret. If continuous mode (CMD) command is input the turret positions 2 and 4 are used for the measurement of unknown samples, and turret positions 1 and 3 can be used to hold monitor samples if required. The changer will then load one sample at a time, and while this sample is being measured any previously loaded sample will be unloaded to its original position in the sample tray, and a new sample from the tray will be loaded.

If the batch mode (BMD) command is input the changer will load as many samples as possible into the sample turret, and then commence measurement of the batch, i.e. unknown samples will be loaded to turret positions 1 to 4 unless a position is occupied by a monitor sample (position protected when the LDM command is given). For example, if the tray contains 6 unknown samples, and there is no monitor in the tray or the turret, the first four samples will be loaded, measured and unloaded, followed by the final two samples.
If a monitor is in turret position 1 then unknown samples are loaded to positions 2, 3 and 4, in two sets of three samples, refer to paragraph 3.2.3. and figure 3.2B.

3.2.7. Monitor measurement

The measurement of a monitor sample will be initiated if the M bit of the identification card is pressed out. This means that the monitor sample in the turret or in the sample tray will be measured. For direct ratio measurements the M bit must always be pressed out, refer to the table 3.2A.

In the buffer ratio mode the M bit will be pressed out only if a monitor measurement update is required. In this case the monitor sample is remeasured (using the SMM routine selected automatically) before the unknown samples are loaded and measured. If the M bit is not pushed out the unknown samples will be measured but the previous monitor measurement and update of buffer results will not take place.

Sample analysis which requires the measurement of a monitor sample can be performed with a monitor loaded into the turret or in position 1 of the sample tray. The monitor sample is loaded into the turret by the LDM command and the turret position is protected against loading any other sample during automatic changer operation until the unload monitor command (ULM) is given. The MP list assembly must show the turret position (MOPS=), see paragraph 1.3.2.

With the monitor sample loaded in the first position in the tray the turret position, specified by MOPS= in the MP list to be used, must be empty. The monitor will now be loaded from the tray to the specified turret position, and will be unloaded into position 1 of the tray after the measurement.

If the measurement program calls for monitor measurement, but a monitor sample is not in tray position 1 or in the turret, an error message is output, the tray is skipped, but the following tray measurements are not inhibited. If the program uses a monitor correctly loaded in the turret (by SMM), any sample in position 1 of the sample tray will be treated as an unknown (non-monitor) sample.

Table 3.2A. Sample changer actions.

Measure mode	*Program card M bit*	*Monitor in spectr. turret*	*Action by changer software*
Absolute	Not M	–	SMX on 6 samples (max.) per tray, BMD/CMD
	M (push out)	–	Error message ** ERROR MONITOR, SMX on 6 samples (max.) per tray, BMD/CMD.
Buffer ratio	Not M	–	SMX on 6 samples (max.) per tray, BMD/CMD
	M	Yes	SMM on monitor in spectrometer SMX on 6 samples (max.) per tray, BMD/CMD *Note: If tray position 1 has a monitor it will be measured as an unknown.*
		No	Monitor loaded from tray position 1, but if position is empty the ** ERROR MONITOR message is output and tray is skipped. SMM on monitor, unload monitor to tray position 1, and 5 (max.) unknowns measured by SMX, BMD/CMD.
Direct ratio	Not M	Yes	SMX (using the monitor in the turret) on 6 (max.) samples in the tray, BMD/CMD.
		No	Error message ** NO MONITOR LOADED IN POS. ... output for each loaded (batch of) samples. No measurement.
	M	Yes	SMX (using the monitor in the turret) on 6 (max.) samples in the tray, BMD/CMD.
		No	Monitor loaded from tray position 1, but if position is empty the ** ERROR MONITOR message is output and the tray is skipped. SMX (using the monitor from the tray) on 5 (max.) samples BMD/CMD. Unload the monitor to the tray.

3.2.8. Regression measurements.

The automatic measurement of samples for use in the regression procedure can be initiated by giving the SPR command (without argument) after the ASC command. All samples up to and including those in the last tray specified by the ASC i command will be measured, and the intensities will be written to a regression file on disc, see paragraph 2.5. If the trays have different measurement programs a regression file will be made for each measurement program.

3.2.9. Recalibration samples

The automatic measurement of samples for use in instrument recalibration can be initiated by giving the SMR, SSR or SAR command after ASC. The manual recalibration procedure requests the input of the number of recalibration standard samples to be used, and the operator must ensure that the same standards are used later in the SSR and SAR routines, and they must be loaded in the same sequence. To avoid any possibility of error it is recommended that recalibration standards are stored in a safe place in the same trays and order as used for the original measurement.

In addition take care that the last tray identification i (in ASC i) is input to guard against too many, or too few, samples being measured in the recalibration routine.

3.2.10. Job measurement

Job measurement can be selected if a job program has been assembled. The job list number must not be the same as any MP list number, therefore it is possible to use the identification card coding to select a job list for sample measurement. If the card has the M bit removed it is disregarded by the software control and measurement proceeds normally.

Note that samples will be loaded one by one to turret position 4 for measurement.

3.2.11. Keyboard controlled operation

All changer operation and sample measurement is controlled from the keyboard. Tray movement (STY i), tray position (MTY i), and loading/unloading the turret (LTU i/UTU i) can be performed, and sample measurement is commenced as paragraph 1 (SMX i, etc.). If required, give RES first to reset the ASC command.

3.2.12. Job controlled operation

Some commands cannot be executed in the ASC mode, but they can be assembled in a job list which is executed when the SJB command is given, refer to paragraphs 1.3.3. and 1.4.7. For example, a monitor sample can be measured by a job list containing STY, MTY, LTU, LDM, SMM, ULM, and UTU, and the various steps will be carried out for the monitor in the changer. The commands marked with ▲ in the list in paragraph 1.2. cannot be initiated from a job list selected by a program card after ASC is given; and any attempt to do so will result in an error message, the sample is unloaded, and the tray is skipped.

3.2.13. Changer description

The sample changer is bolted to the front of the spectrometer, and is aligned as described in the Service Manual. Tray movement in a fore and aft direction is by means of four motor driven belts (two in each direction), and the side movement (front side and spectrometer side) is by means of two independently motor-driven discs which engage with the trays. The position of the trays are signalled to the control circuits and microprocessor by the operation of various microswitches. If defined tray positions are not reached within predetermined times the operation is inhibited and an error message will be output. The grab arm mechanism is identical to the sample loader, i.e. the horizontal movement and vertical movement cams are motor operated, and microswitch operation signals the arm position. The main control circuit is fitted in the right-hand side of the spectrometer, and a light-beam detector is fitted at the sample loading hole.

A matrix of infra-red sensors detect the coding of the tray identification card.

3.3. PW 1464/50 HELIUM SYSTEM

The PW 1464/50 system will maintain a helium gas atmosphere in the spectrometer chamber and in the sample loading position, when selected. This enables the analysis of light elements in liquid samples which is not normally possible with a vacuum or an air X-ray beam path.

3.3.1. Operation

The helium system should be connected as figure 3.3A. The valves at the gas bottle should be opened, and the regulating valve on the flow meter assembly of the right-hand side panel should be adjusted to a flow of approximately 60 litres per hour.

The VACUUM/HELIUM/AIR push-buttons on the front panel must all be in the released (out) position before any one of them is operated.

All air should be evacuated from the spectrometer chamber (VACUUM push-button depressed), before selecting a helium atmosphere (release VACUUM then depress HELIUM).
If accurate measurement of light elements is required the process should be repeated, i.e. VACUUM, HELIUM, VACUUM then HELIUM atmospheres selected.

It is suggested that the heavier elements are analysed first so that any air in the chamber will have been flushed out by the time that the light elements are measured. Sample analysis is performed in the normal manner, and after a sample is loaded and the cap is down a flow of helium gas will flush the air from the loading position.

After using the helium system the HELIUM push-button should be released, and if further analysis is in an air or vacuum atmosphere the valve at the helium gas bottle should be closed.

3.3.2. Description

The operation of the valves in the helium gas system is controlled by the microprocessor software, refer to the flow diagram figure 3.3B. The HELIUM selection push-button on the front panel is the only operational control, the side panel flowmeter indicates the gas flow, and the gas flow regulator is situated just above the flowmeter.

3.3.3. Adjustment and maintenance

The adjustment, as mentioned above, is to set the flow rate to a suitable value, normally around 60 litres per hour.

The only maintenance necessary is to change the gas cylinder when it is empty. This procedure is similar to the description in paragraph 6.2.3. for the detector gas system, except that the coupling nut has a right-hand thread and must be turned counter-clockwise to loosen.

Check for gas leakage, as described in paragraph 6.2.3.

The gas used for the Helium system should conform to the following:

Volume per cent	He	=	99,995%
Impurities:	N_2	<	10 ppm
	O	<	1 ppm
	H_2O	<	10 ppm
	H_2	<	0,5 ppm
	CxHy	<	0,1 ppm
	Ne	<	10 ppm
	CO_2	<	0,5 ppm

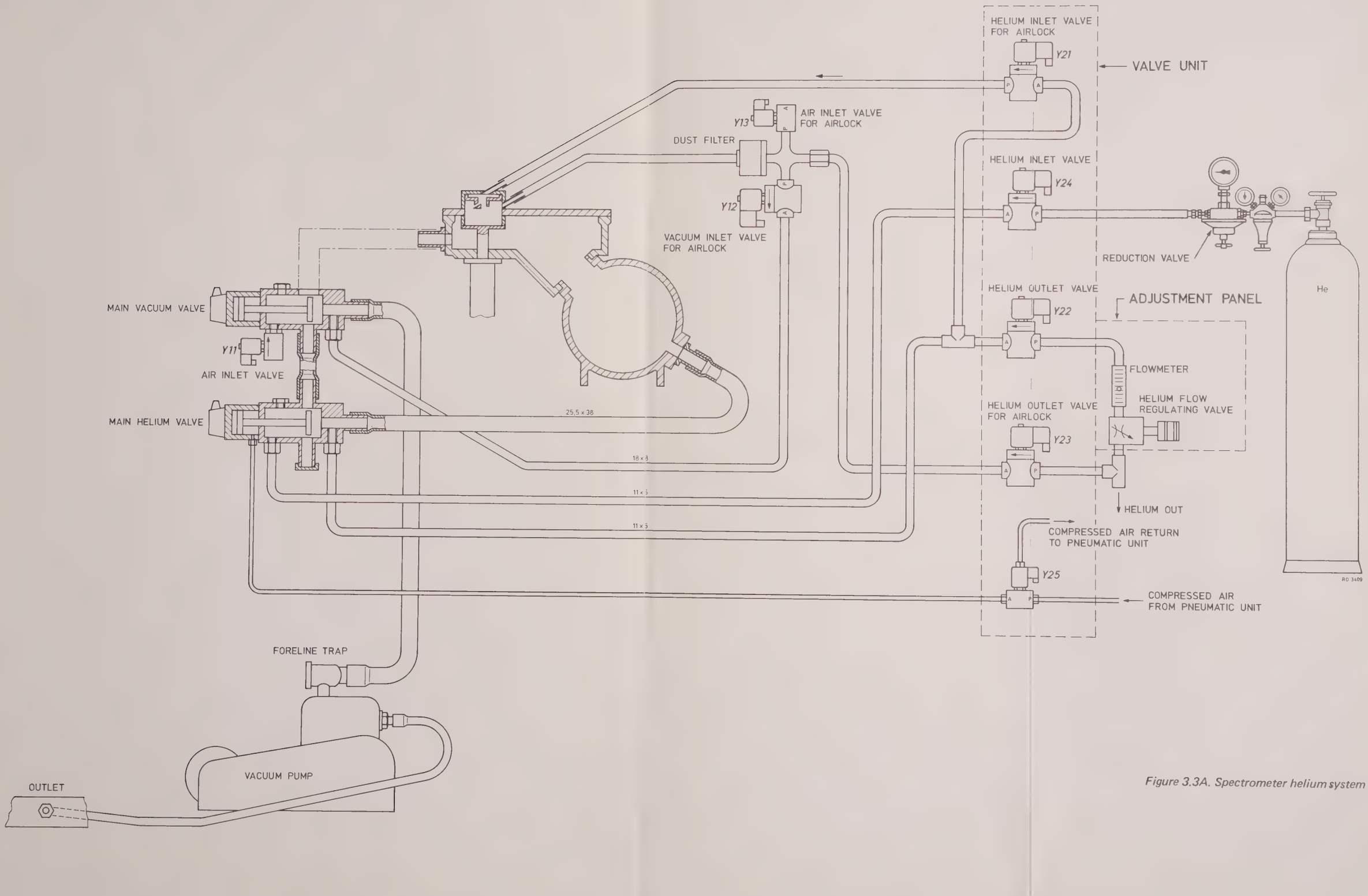


Figure 3.3A. Spectrometer helium system

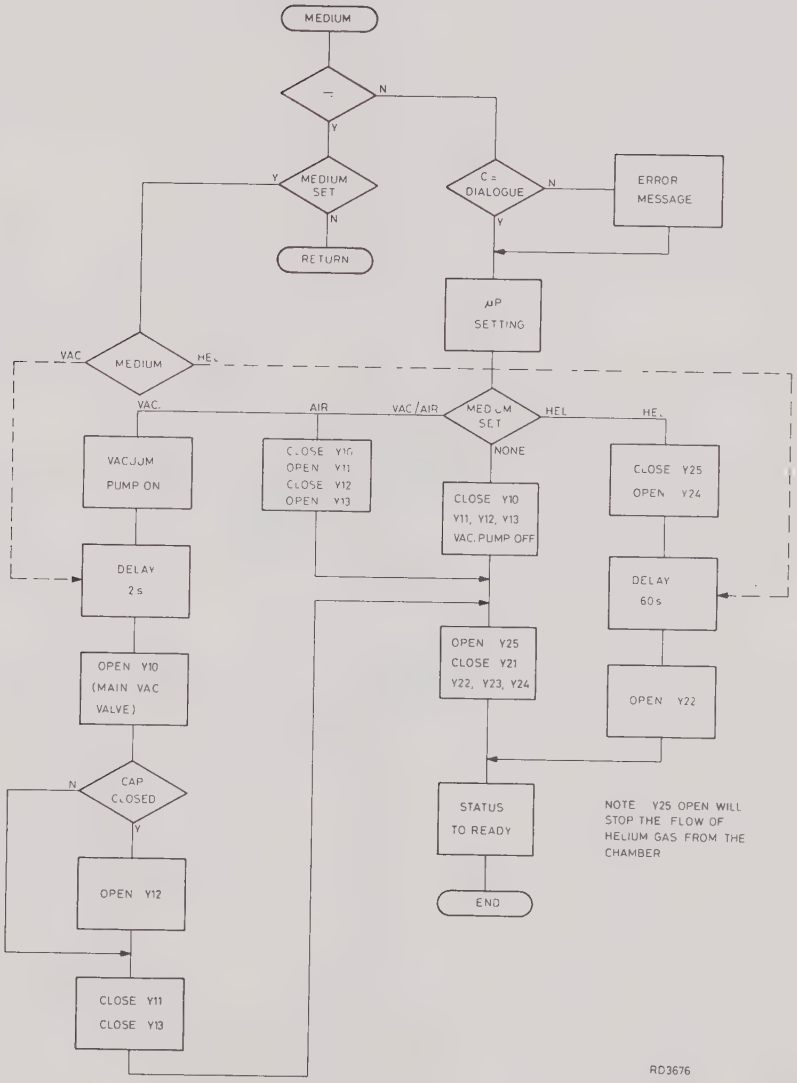


Figure 3.3B Spectrometer medium selection flow chart.

3.4. PERIPHERAL DEVICES

3.4.1. General

The flexible input/output interface fitted in the PW 1400 is capable of connection to the devices mentioned in this paragraph, or to a computer, such as the Philips P851. When a computer is connected, the input/output peripherals will normally be connected to interfaces which are part of the computer equipment.

The devices which can be connected in a PW 1400 system are shown in figure 3.4A.

The facilities available by jumper selection on the interface card are best selected to suit the analysis requirements. These facilities (baud rate, duplex/half duplex working, echo, parity check, bits per character, etc.) will be set at installation, and if the type of peripheral is subsequently changed refer to the Service Manual for details of the connection and jumper settings.
The jumper and switch settings of the peripheral circuits (internal) will also be found in the Service Manual of the PW 1400 or in the peripheral manuals.

The following sub-paragraphs describe the three main peripherals which can be connected to the PW 1400 or P851 computer, and the necessary keyboard operations.

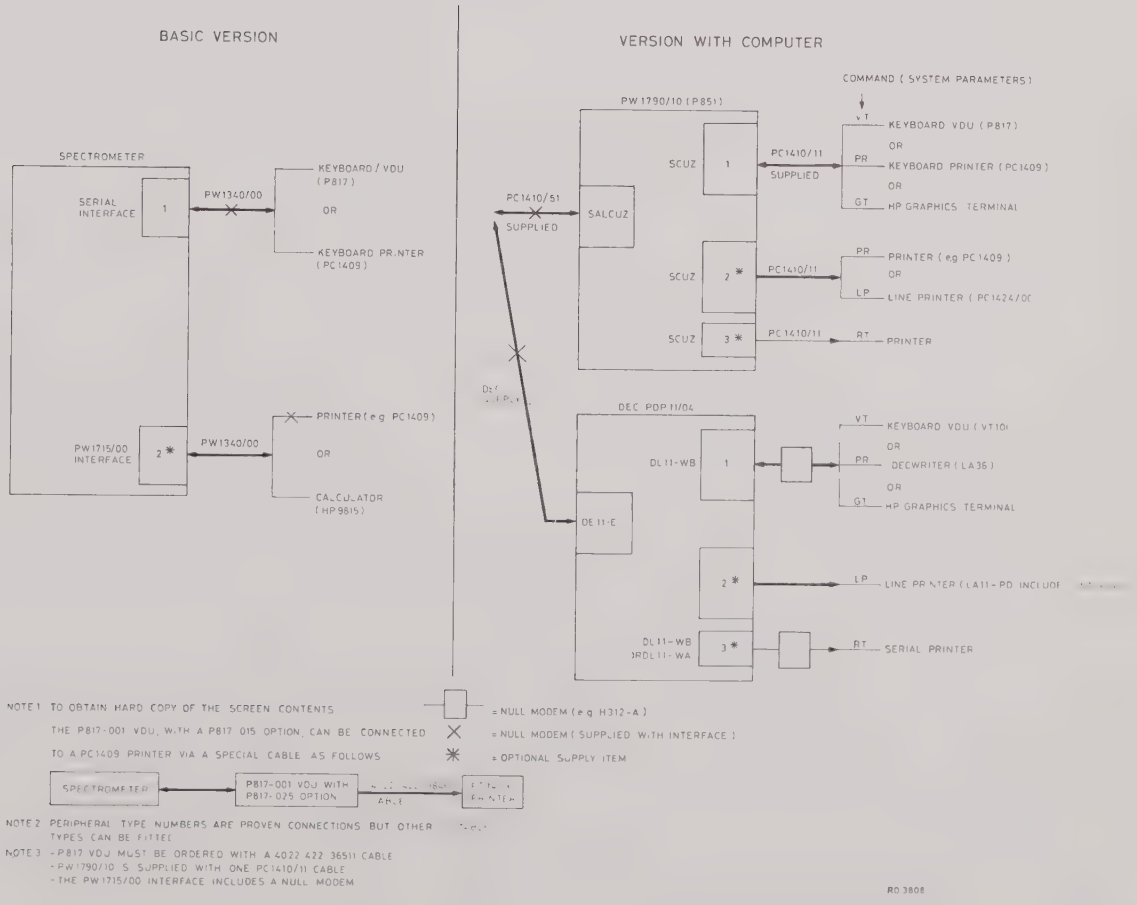


Fig. 3.4A. Possible peripheral connectors

3.4.2. PC 1409/00 Character printer

The printer has a matrix print head mechanism, and will deliver a true 30 character per second throughput upper and lower case printing, and 132 column format on 28 cm (11 inch) wide fan-fold paper. A layout of the printer keyboard is shown in figure 3.4B.

For normal operation the upper key-switches DATA, PARITY and DUPLEX must be depressed, and the other keys should be normal (up). For the normal typing of data (off-line operation when the spectrometer is not in use) the LOCAL key should be depressed.

On the main keyboard the CAPS LOCK key must be depressed, otherwise an error message will be printed if software commands are typed.

3.4.3. P817 Video display unit

The P817-001 display unit has a 12 inch diagonal CRT screen to display up to 24 lines of 80 characters. The number of lines (per page) for display is set by the NRL i command, see paragraph 1.5.2., and if i = 0 the data appears at the bottom of the screen and moves upwards as new data is input. This unit can only be used to display output data, i.e. connected to the second interface, but it can be used as the main terminal if a keyboard option is supplied.
An on/off mains switch is at the lower right-hand of the screen, and a brightness control is underneath the front of the unit.

The optional P817-052 is an alpha-numeric keyboard which will enable the VDU to be used is a main terminal, if required.

For normal operation the RDY lamp should be lit, and on the main keyboard the CAP lamp should be lit (if not operate the CAP key).

3.4.4. HP2648A Graphics Terminal

This terminal has a screen (5x10 inches) with a capacity of 24 lines of 80 characters, a 128 alpha-numeric character set, and a memory of 8k bytes for alpha-numeric display and 32k bytes for graphical display (720 dots x 360 rows of displayable points).

Facilities exist for the selection of the data (baud) rate, transmission mode, operating mode and parity check, and details will be given in the manuals supplied with the terminal.

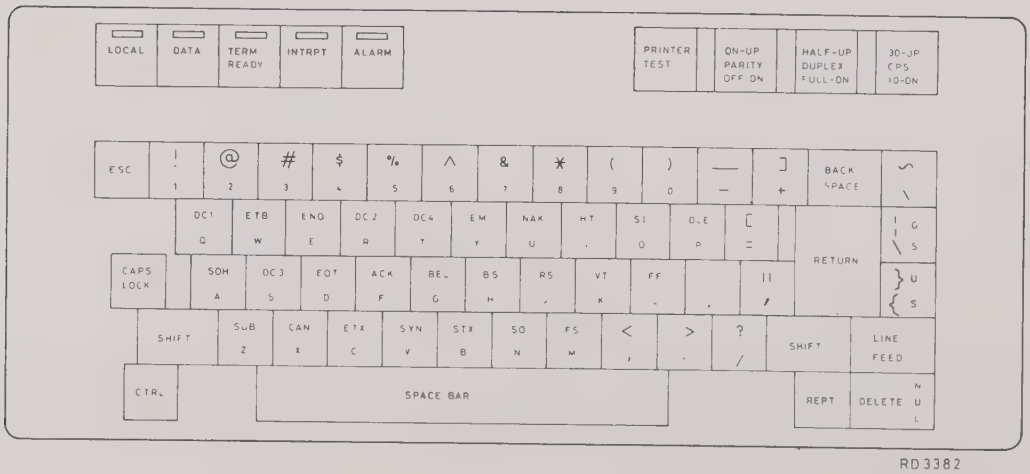


Figure 3.4B PC1409 Printer keyboard layout

4. ANALYSIS INFORMATION

4.1. GENERAL

The following notes should be observed before and during analysis:

1. The spectrometer must always be connected to a live electrical mains supply, even if the system is switched off. In this situation the spectrometer temperature stabilisation is operational, and the microprocessor memories are active. In the event of power failure a battery mounted on the bus interface card will protect the memory contents for one month under worst case conditions. The battery switch must be on, and the battery must have had two charge/discharge cycles - see the Service Manual.

   The temperature stabilisation system is adjustable from about 25 °C to 35 °C, and the maximum time required for stabilisation is 6 hours when the mains supply is connected.

2. Before switching the system on ensure that:
   - the water supply is connected and turned on
   - the detector gas system is operational
   - the helium gas system is operational (if installed)
   - all doors are closed and covers fitted
   - the HT generator controls kV and mA are in the minimum position
   - check that the cap (loading position) is down
     the loose (PW1160/00) X-RAYS ON warning lamp is connected.

3. When the system is switched on (by the MAINS I push-button on the HT generator), check the following:
   - the HT to the flow and scintillation detector is correctly set
   - the computer is working, the XR1400 diskette is loaded and the programs are running
   - the peripheral devices are matched to the interface(s)
   - the correct terminal, output device(s) and parameters are selected by the ASP command
   - the maximum limit for HT generator output power selection and kV selection should be set by the PWR command.
   - any other system conditions should be correctly set, e.g. spinner (SPN), collimator mask (MSK), etc.

Note that the PWR and SPN commands remain active if the system is switched off and on.

4. When the generator HT is switched on (by the HIGH VOLTAGE I push-button), and before measurement commences, ensure that:
   - the water, gas, and temperature systems are operating satisfactorily
   - all X-RAYS ON warning lamps are lit.
   - when an X-ray tube has been changed, or the water hoses have been disconnected for any reason, the HIGH VOLTAGE I and 0 push-buttons should both be held depressed for a few seconds to flush any air bubbles out of the system.
   - do not switch off the HT if high precision is required after a period of non-use (overnight or week-end), refer to paragraph 1.1.1.
   - if the X-ray tube is new, or it has not been used for long period, the generator high-voltage and current should be applied gradually - see paragraph 6.5.1.

5. Input commands such as SPN, MSK, BMD/CMD, recycle, etc., before commencing the analysis.

6. If an analysis must be interrupted give a stop command - see paragraph 1.2.

7. Refer to the notes in paragraph 1.1.1. before turning off the electrical, water, or other supplies to the spectrometer.

4.2. SAMPLE PREPARATION

4.2.1. General

Where special problems are encountered, the advice of N.V. Philips' Application Laboratory should be sought, preferably via the local Philips organisation.
Reference is made to four types of sample in this manual, defined as follows:

(i) *Unknown sample* — is a sample whose elemental composition is not known and requires determination by measurement at selected 2θ angles.

(ii) *Standard sample or calibration standard* — has an accurately known (and usually certified correct) chemical concentration of each element. A series of these samples will be used to calibrate the spectrometer.

(iii) *Recalibration sample* — has an accurately measured, or calculated, apparent concentration, i.e. the measured intensity will be corrected for dead-time, background and line overlap effects. Recalibration samples are used to quickly determine whether any change of the characteristics of the spectrometer have affected the D and E calculation constants.

(iv) *Monitor sample or ratio standard* — has the characteristic of being stable for a long period of time, for a particular element or elements. Measurements performed in identical conditions should give repeatable results, and any change in the measured element intensity will indicate a change of characteristic of the spectrometer.

It should be noted that if the sample is a magnetic material, there will be interference with the electron beam from the X-ray tube and some inaccuracy of measurement will result.

For liquid a titanium cell covered with mylar foil is available for measurement in air atmosphere, with an optional holder for measurement in a helium atmosphere.

Specimens for X-ray analysis should be effectively infinitely thick, i.e. solid specimens should be approximately 3mm thick. Once the specimen has been prepared care should be taken that it fits into the holder properly.

Up to four prepared samples can be loaded into the spectrometer, including any monitor samples. If a sample changer is installed it is possible to load samples which can be analysed using different measuring programs.

4.2.2. Non-metallic powder samples

Many samples which have to be measured in the spectrometer will be in the form of powders (cement raw materials, ores, soils, slags, geological samples etc.).
The following preparation methods can be used:

- *Direct pelletizing*

  The materials as received are pressed into pellets (preferrably using aluminium cups PW 1527/81).
  This is only possible if the material received is of sufficiently small and constant grain size.

- *Grinding and pelletizing*

  This is the generally used method. The sample is placed in a vibrating-disc type mill such as the Herzog HSM 100 and ground for a predetermined length of time.
  Then a tablet is pressed from the ground material. By always grinding for the same length of time and by always pelletizing at the same pressure and holding that pressure for the same time for all pellets, very consistent samples can be prepared. There are several variations of this method such as:

  a) Adding a binder to the material after grinding in order to obtain a stronger pellet. This can be done in various ways, two of which are described here. With the first method the ground material is mixed with a wax type binder (such as Hoechst Wachs C), and the sample is pelletized. The wax flows and holds the particles together. A reasonably strong pellet is obtained in this way.
  In the second method a number of drops of a 1:5 solution of n-butylmethacrylate in acetone is mixed with the ground material in a mortar and then allowed to dry. Then it is lightly ground in the mortar (a few seconds suffices). The material is now put into the press and pelletized. The binder polymerizes under pressure and a very strong pellet is obtained. This second method takes a little time but gives extremely strong pellets and is highly recommended.

b) Adding a binder/grinding aid to the sample during the grinding (SOMAR MIX, HEA 2 etc.).
This method has two important advantages. Firstly the additive will act as a grinding aid which means that a smaller and more uniform particle size is obtained in a given time than with dry-grinding. Secondly it distributes the binder (usually a soapy type material) very finely through the sample so that after pelletizing a strong tablet is obtained.

c) Using the wet grinding technique. This method has been tried on a number of cements and is found to give an extremely small grain size almost completely overcoming particle size effects.
The method is as follows:
In a 100 cc grinding vessel (test carried out on a HSN 100) 50 grams of powder (cement) is placed and 25 cc of isopropylalcohol are added. The grinding vessel is then closed and the material ground. Some results: sieve test on a 20 micron sieve after 5 minutes grinding 1.5% i.e. 98.5% of the grains are smaller than 20 microns. Al-intensity stable after 3 minutes. Fe-intensity stable after 1 minute. Si-intensity stable after 4 minutes. After grinding be careful when taking the lid off the grinding vessel. The temperature in the vessel may have reached the flash point of the alcohol and spontaneous combustion may occur. This does not matter at all and the sample will dry rapidly. It can then be pelletized in the usual way.

- In some instances, notably where the mineralogical composition of the sample is variable (that is the desired element is present in several mineralogical forms and the ratio between these is not sufficiently constant), none of the above methods may render sufficiently accurate results. Then there is no option to destroy the minerals. Two ways are possible.

- *Liquid solution technique*

  The sample is dissolved in a suitable acid. The method is often rather time consuming (unless the "bomb" technique is used) and it may be necessary to use some very strong acids.
  However, the introduction of such acids in the spectrometer should be avoided wherever possible.

- *Solid solution technique*

  Here a weighed amount of sample material is mixed with a weighed amount of flux (lithiumtetra- or meta borate, sodium meta- or tetra borate etc.). The mixture is heated in a crucible to 1000 - 1400°C and the sample and flux together form a homogeneous glass bead. Heating can be done in graphite, gold, platinum, platinum/gold or platinum/rhodium crucibles in a muffle furnace, over a Bunsen burner, by RF heating, etc. There are possibly hundreds of recipes all over the world.

4.2.3. Metal powder samples

By metal powder is meant drillings, filings, shavings etc. that can be obtained from large pieces of metal. The following methods are generally used:

Analysis of loose drillings or filings stuck to adhesive tape. Not a commonly used method.

- *Pelletizing*

  Very frequently it is possible to pelletize shavings of the softer metals such as aluminium and its alloys, lead and tin alloys, solders, gunmetals etc. The ensuing pellet can be put into the spectrometer.
  In general quite high pelletizing pressures are required. Herzog HTP 150 up to 150 tons pressure.

- *Acid solution technique*

  Usually it is easier to get metals into solution than powders. The same advantages and disadvantages apply as mentioned under *"Liquid solution technique".*

- *Remelting*

  Metal shavings etc. can be remelted, cast and the resulting casting treated as a solid sample.
  Usually either a vacuum or a protective atmosphere type furnace is needed and melting can be done with electrical arc or RF heating (suppliers of this type of equipment are M.B.L.E., Edwards High Vacuum, Pitchford Scientific Instruments etc.).

4.2.4. Solid metal samples

This preparation procedure can be split into two parts:

1. preparation of samples taken from the melt
2. preparation of samples from round or square stock, ingots, sheets etc.

1. Preparation of samples taken from a hot melt. The hot metal will have to be cast in a mould, either a normal one or a water cooled one for chillcasting. The sample is then cut into two pieces and the surface is finished. Surface finishing can be carried out on a lathe, a circular sander with emery paper or a belt sander. Sometimes polishing with diamond paste is necessary.
   Care should be taken that no smearing takes place when treating the sample surface. The preparation of the sample should not introduce any contamination due to the grinding agent, lubrication, finger marks etc. and the storage of the sample before measurement should not introduce contamination due to moisture, hydrogen sulphide, sulphur dioxide etc.. Spinning the specimen will even out any irregularities due to surface finish, slight inhomogeneities and differences in primary X-ray intensity.

2. Samples prepared from round or square stock, ingots, sheets etc.
   Usually these samples will have to be brought to the correct size for the spectrometer.
   Surface treatment is then identical to that given above.
   It should be noted that if the specimen is a magnetic material there will be interference with the electron beam from the X-ray tube and some inaccuracy of the measurement will result if the magnetic properties of the unknown specimens differ from the calibration standards.
   References to useful literature on the preparation of samples etc., can be found in the Review of Literature XRF, published regularly by N.V. Philips.

4.3. SAMPLE HOLDERS

4.3.1. General

The range of sample holders is shown in figure 4.3A., and these are intended for use as shown in table 4.3.1. The viewing circle of the collimator masks which are available are shown in figure 4.3B., and note that only two masks can be fitted in the PW 1400, selected by command MSK i, where i = mask 1 or 2 (DIAPHRAGM on front panel display). The reduction in intensity is shown in figure 4.3B., where 100% is the intensity without a mask. The mask chosen for use should have a smaller area than the aperture of the sample holder. Samples for use in a sample changer should not exceed a weight of 400 grammes per sample.

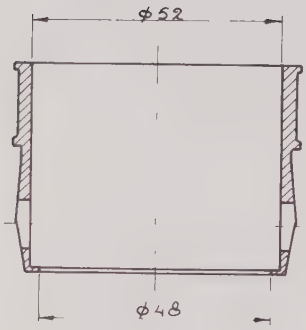
Table 4.3.1. Sample holder details

TYPE OF SAMPLE	TYPE NUMBER	BOTTOM APERTURE		DIAMETER OF PLASTIC INSERT
		DIAMETER OF OPENING	MATERIAL	
50mm ϕ SOLID	PW1427/50*	48mm	ALUMINIUM	
40mm ϕ SOLID	PW1427/54* PW1427/64	37mm 37mm	ALUMINIUM COPPER	41mm 41mm
32mm ϕ SOLID	PW1427/53* PW1427/63	30mm 30mm	ALUMINIUM COPPER	33mm 33mm
32mm ϕ BEADS	PW1427/62*	26mm	COPPER	33mm
LOLLIPOPS OR OTHER IRREGULAR-SAMPLES	PW1427/50* PLUS PW1428/25 or /30	25mm or 30mm	GOLD GOLD	LOLLIPOP SIZE
5mm to 25mm SMALL SAMPLES	PW1427/50* PLUS PW1428/01	5mm to 25mm CUSTOMER DRILLS HOLE TO REQUIRED SIZE	COPPER	25mm
LIQUIDS IN HELIUM OR AIR	PW1527/90 PLUS PW1427/91	42mm	TITANIUM CELL ALUMINIUM	
LOOSEPOWDERS IN HELIUM OR AIR	PW1527/90 PLUS PW1427/91	42mm	TITANIUM CELL ALUMINIUM	

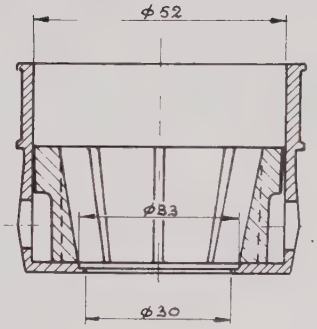
* Sample holder to be used with collimator mask

Notes:

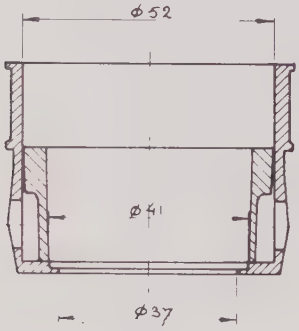
1. Lollipops: The PW1428/25,30 or 37 are special gold-plated masks that fit the PW1427/00 for use in the analysis of irregular-sized samples, between 25mm and 37mm, which do not allow the use of collimator mask and for which a copper mask cannot be used as its influence will be unacceptable. It is also used for the analysis of "Lollipops" in the Steel Industry.
2. PW1527/90: A titanium cell used in the analysis of liquids and loose powders both in helium and air
3. Copper Masks: Where copper masks are mentioned it should be realized that these masks are not pure copper but contain 0.4% - 0.7% tellurium besides copper.



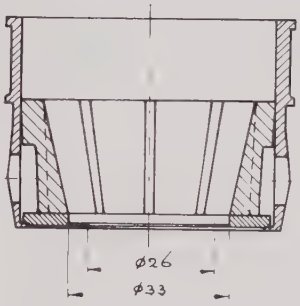
PW 1427/50
Quantity = 10



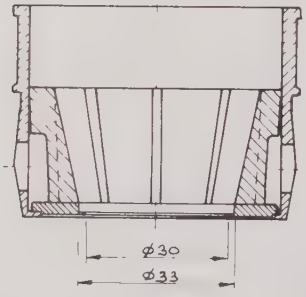
PW1427/53
Quantity = 10



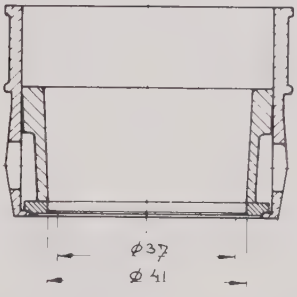
PW1427/54
Quantity = 10



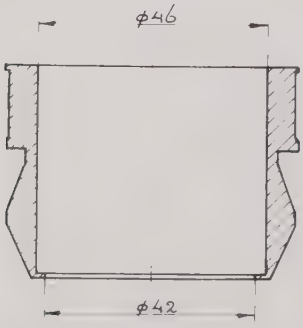
PW1427/62
Quantity = 10



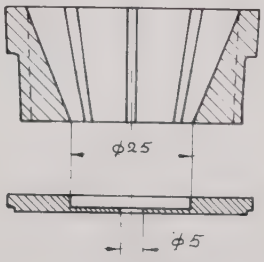
PW1427/63
Quantity = 10



PW1427/64
Quantity = 10

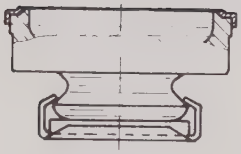


PW1427/91
Quantity = 5

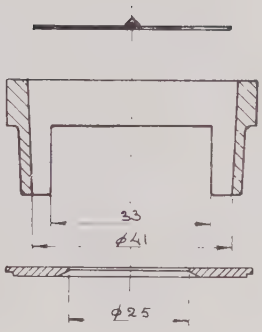


PW1428/01
Quantity = 10

Fig. 4.3A. Sample holders and masks



PW1527/90



PW1428/25

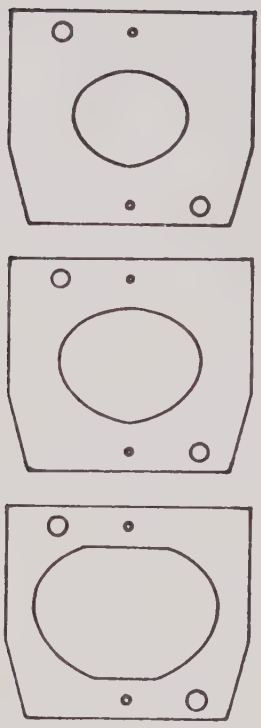
PW1428/30

PW1428/40

Fig. 4.3A. Sample holders and masks

car plugs

natural plastic



collimator masks as used in PW1400

EFFECT ON INTENSITY

MASK	INTENSITY
none	100
35 mm	90
28 mm	80
24 mm	60

Fig. 4.3B. Viewing circle of collimator masks

4.3.2. PW 1527/90 Cell for liquid samples

A special cell with a mylar film window may be used to hold liquid samples for analysis.
Liquids, provided that they are single phase and relatively involatile, represent an ideal form for measurement, where the vapour pressure of the liquid to be analysed is too high to allow the use of a vacuum path and a helium path (or air) must be used.

The liquid cell consists of three parts, a body, a clamping ring, and a sliding seal.
A piece of thin Mylar foil (PW1526/00) is stretched and trapped between the clamping ring and the cell, the cell is filled with the liquid to be analysed, and the seal is applied to the fill opening.

Although the liquid cell may be used for loose powder samples this procedure is not recommended unless it is unavoidable.

The cell is prepared for use as follows:

1. Place the clamping ring on a clean flat surface with its flanged face downwards.
2. Lay a piece of Mylar foil (approximately 10x10 cm) over the clamping ring.
3. Place the stretching ring (external diameter 60mm, height 4.5mm) on the foil and stretch the foil by pulling at all four sides.
4. Push the liquid cell into the clamping ring while firmly pressing down on the stretching ring.
5. Remove the stretching ring and examine the liquid cell to ensure that the Mylar foil is stretched smoothly.
6. Cut the excess foil from the rim of the cell.
7. Place the cell on a clean level surface and fill it with the liquid to be analysed. Ensure that the surface of the liquid is slightly higher than the rim of the opening.
8. Close the cell by carefully sliding the seal over the opening until it is firmly in place.
9. Check the cell for air bubbles. If any bubbles are observed, refill the cell and check again.
10. Place the cell in a sample holder and analyse it in the usual way using air, vacuum, or helium as appropriate.

CAUTION

As a general rule do not use vacuum for analysing liquids because the mylar foil may rupture and damage to the spectrometer may occur. If the required measurement precludes the use of an air path, then helium must be used.

A special tool set PW 1527/91 (consisting of a key and a ring with a diameter of 50mm and a height of 9mm) is provided for removing the clamping ring and the Mylar foil after the cell has been used for a measurement. To remove the foil proceed as follows:

11. Pour the liquid out of the cell.
12. Place the cell on a flat surface (Mylar foil downwards) and place the ring over the cell so that its rests on the clamping ring.
13. Using the key as a lever, separate the cell from the clamping ring.
14. The cell may now be cleaned ready for reuse.

4.4. PULSE HEIGHT DISTRIBUTION SCAN

4.4.1. General

A pulse height distribution record enables the choice of the best settings of the pulse height selector circuit (LWL and UPL), and it can be used to determine the resolution of a detector (see paragraph 4.4.3.). The PHD record can be obtained as described in paragraph 1.4.11., or by using the computer to obtain a printer bargraph, or display on a VDU or graphics terminal. Note that the computer can calculate the value of detector resolution, and output a percentage value.

A pulse height distribution command can be given to produce a printer readout or a chart recorder record after a measurement. Both commands will select element measurement parameters, but the lower level and upper level program values are not used except to make an initial measurement. The PHD command includes a window width (UL minus LL) argument, and for a printer output the time per step measurement must be given. The readout in figure 1.4R. shows the distribution of counts as the lower level is progressively stepped from 0 to 100%. In the manual mode the microprocessor will readout a listing of count values.

Output to a chart recorder is given when 0 (zero) is input to the command time input request, see figure 1.4S. In this case the lower level is continuously varied from 0 to 100%.

Another form of readout can be given by a graphics display unit, as shown in figure 2.4S., and described in paragraph 2.4.10.

Referring to figure 2.4R. the computer readout will show the bargraph, followed by the element channel and window width (as input with PHD) , the situation of the element peak (MAXIMUM = generally around 50%), the calculated resolution of the detector system (see paragraph 4.4.3.), the date and time, and the countrate using the channel set lower level (LWL =) and upper level (UPL =) values (from a preliminary measurement of 1 second).

The pulses from the detector pass via a pre-amplifier to a correction amplifier which varies the pulse amplitudes. The correction is dependent on the setting of the ATTENUATOR (right-hand side panel), the sine theta potentiometer, the selected crystal and order of reflection, and a pulse shift correction circuit. The pulse shift correction circuit ensures that the integrated number of pulses below the 50% lower level value are equal to the total pulses above 50%.
A push-button CALIBRATE will disable the pulse shift correction, for example to permit adjustment of the H.T. to the detectors. The output from the correction amplifier goes to the main (fixed) amplifier and then to the pulse height discrimination circuit.

The discriminator circuit will block those pulses which are below a lower level (set by LWL =) and above an upper level (set by UPL =). The setting of the lower and upper levels should be selected to count only those pulses which are due to the element peak, and to discriminate against low amplitude pulses due to electronic noise, and pulses due to interfering elements.

4.4.2. Recording a pulse distribution scan

Impurities in the counting gas will cause the flow detector to become contaminated, and its performance will change. The change results in lower pulse heights and a broadening of the pulse height distribution curve, and the measurement results will be adversely affected.

The pulse height distribution of the system should be regularly checked, e.g. for CuKα, and if the resolution is greater than around 20% for CuKα at 20 000 counts per second, it can be assumed that the counter requires cleaning and the counter wire should be replaced, refer to paragraph 6.2.

An automatic pulse height distribution scan can be made with the PM 8203 Chart recorder, as follows:
- Insert the sample in a holder and bring to the measuring position (SLP i, SMP i).
- Assemble a channel set for the element (ACH), if not already existing.
- On the recorder:-
  Put switch "▼" in the upper position, switch "CHART DRIVE" on the left hand side to "8cm/min" and "CHART DRIVE" on the right to "INT".
  If required, transport the recorder paper until the recorder pen is on a line. This is done by putting switch "▼" for a short time in the lower position.
- Give the command PHD xxi , and reply to WINDOW = and TIME = 0 (i.e. for chart recorder output).

The resulting curve should be similar to figure 1.4S.

The figures 4.4A. and 4.4B. show the relation of the pulse distributions for CuKα for the flow detector and the scintillation detector.

It will be seen that the distribution curve for the flow detector is more narrow than the curve for the scintillation counter.

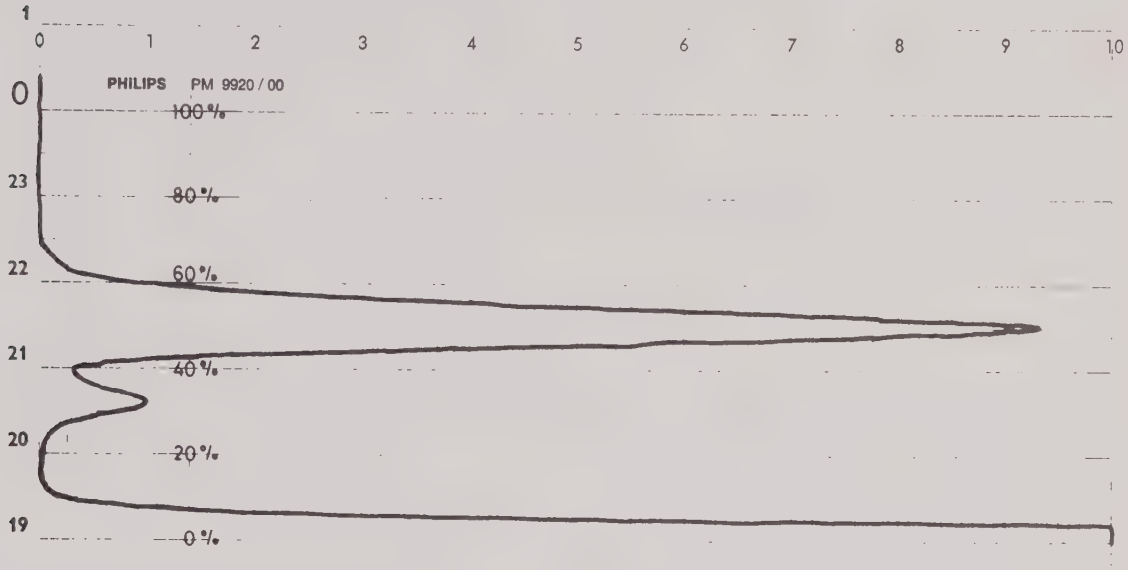


Fig. 4.4A. Flow detector distribution curve for CuKα

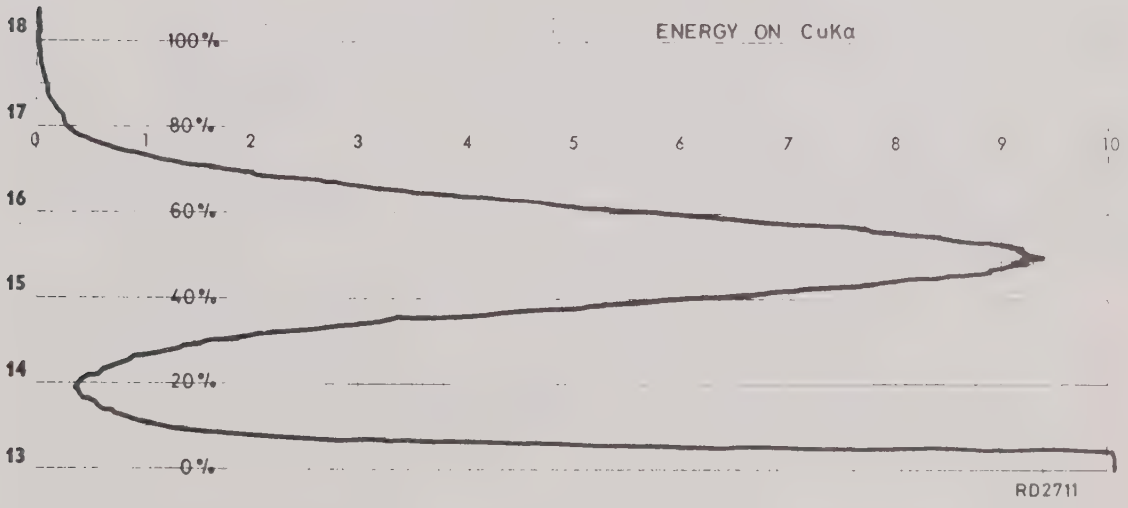


Fig. 4.4B. Scintillation detector curve for CuKα

4.4.3. Determination of a detector resolution

To calculate the resolution of the flow detector and the scintillation detector, the maximum height of the peak is determined and the width of the curve at half this maximum height (known as full width at half maximum, FWHM) is measured. The resolution is calculated from the formula:

$$\text{Resolution } R = \frac{\text{FWHM}}{V} \times 100\%, \text{ where } V = \text{average peak height, and this value is wavelength dependent.}$$

The theoretical resolution for the flow counter is given by:

$$R = 0{,}383/\sqrt{E} = 0{,}109\sqrt{\lambda}, \text{ where } \lambda \text{ is the wavelength of the element line.}$$

By dividing the printed resolution by $\sqrt{\lambda}$ a quality factor Q can be derived, and will be constant for every radiation measured with a particular counter.

Typical values of factor Q are:

Detector	*Q factor*
Flow counter	11 (i.e. 0,109 x 100)
Scintillation counter	44

If a measured quality factor (Q) is much larger than the values given above, and if the resolution of a counter is important because of interference effects, the flow counter should be cleaned and other types of counter replaced.

4.4.4. Selection of preset windows

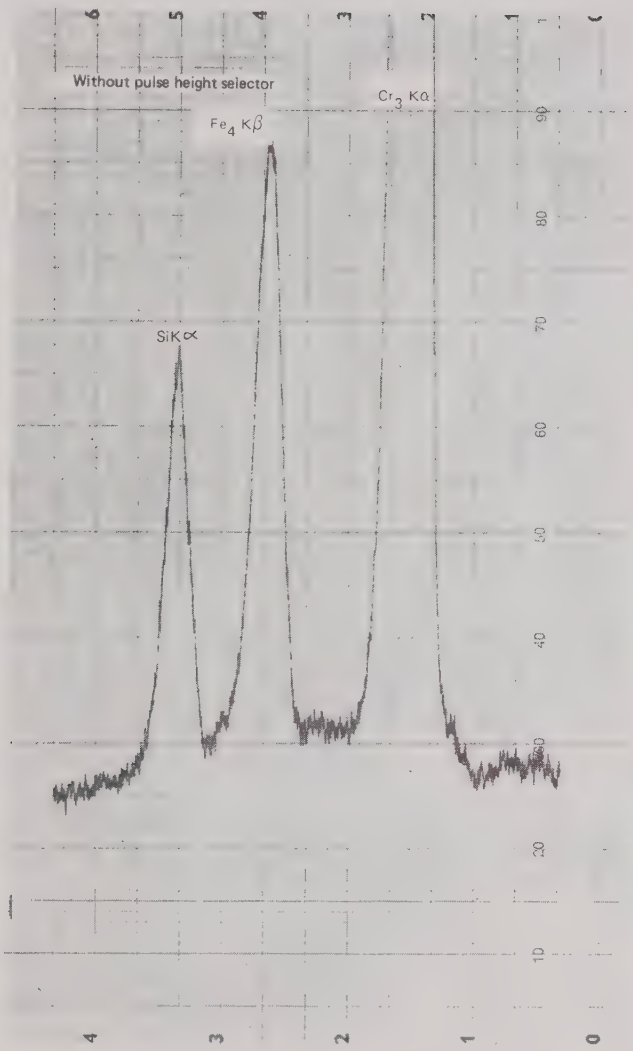
With the aid of a pulse distribution scan, taken for the various elements in the measuring programme, a careful selection can be made of lower and upper level so that only those pulses which are due to the element of interest will be accepted for counting. With this selection it must be considered that the "lower level" and "upper level" settings must be in such a way that:

- the whole escape peak is either inside or outside the window (include if possible)
- do not set the levels too close around the peak
- levels are set wider for the scintillation detector, and narrower for the flow detector
- in trace analysis of light elements a narrow window will improve the peak to background ratio
- the ratio is also improved with a narrow window for higher order interferences, e.g., Ca on Mg.
- take care of the escape peak for elements Ti to Mn.

The effect of a careful selection is illustrated by figure 4.4C. where a steel specimen is measured with a) a lower level set to 10% and the upper level to infinity, and b) with the lower level at 30% and the upper level at 70% (window = 40%).

The SiKα line at approximately 109° 2θ is the element line of interest and its net count rate (above the background level) is virtually unchanged in two recordings. The most obvious effect of applying pulse height selection is that the background is considerably reduced and the spurious peak due to the 3rd order Cr is substantially attenuated and the 4th order Fe peak has disappeared.

(a) LL = 10% , UL = ∞



(b) LL = 30%, UL = 70%

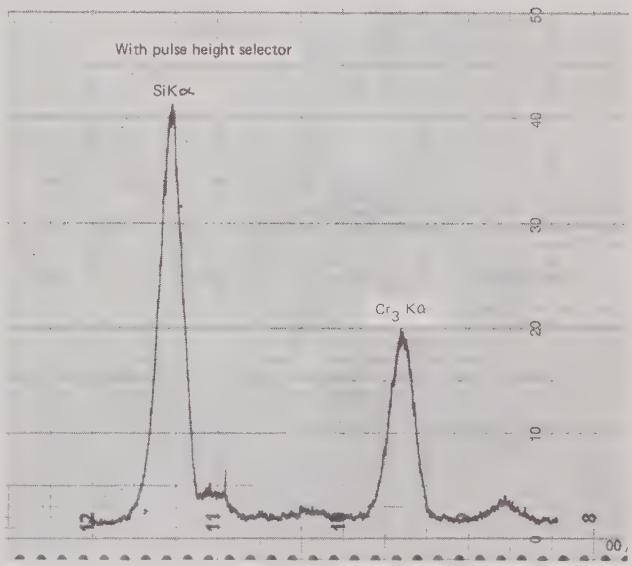


Fig. 4.4C. Effect of pulse height selection

5. SYSTEM DESCRIPTION

The basic PW 1400 Spectrometer system comprises three main units – the spectrometer cabinet, the H.T. generator, and an input/output terminal. The basic system can be extended with a PW 1790/10 computer cabinet, and these units are described in this paragraph.

5.1. BASIC SPECTROMETER UNIT

The spectrometer cabinet contains the spectrometer chamber with crystal changer assembly and detectors, the goniometer, X-ray tube, sample turret with loading position and sample spinner, vacuum system, pneumatics, temperature stabilisation system, gas system for the flow detector, optional helium gas system, control and safety circuits, and power supplies.
There is a display and control front panel adjacent to the sample loading position, various preset controls and indicators underneath the top right-hand side panel, and a lower electrical rack at the rear of the cabinet. The right-hand side panel has plug-in circuit boards, which include the microprocessor circuits, programmable read only memories and random access memories, required to operate the system as described in paragraph 1.

The rear panel (figure 5.1A.)allows connection of the following:

- Connector to the H.T. generator rear connector
- Connector to the terminal peripheral (1)
- Connector to the output only device (optional)
- Connector to a chart recorder (if required)
- GAS ARGON ↑ IN for the gas-flow detector
- GAS HELIUM ↑ IN ↓ OUT, when a helium gas system is installed
- COMPRESSED AIR ↑ IN ↓ OUT, for the pneumatics system
- VAC PUMP EXHAUST, from the vacuum pump (if required)
- COOLING WATER ↓ OUT, ↑ IN — TUBE — X-ray tube cooling circuit.
- COOLING WATER ↑ IN, ↓ OUT — CABINET — Temperature stabilisation system.

In addition there is access at the rear for the 220 volts mains supply to the H.T. generator, the H.T. cable to the X-ray tube from the H.T. generator, and the wiring to the X-RAYS ON lamp assembly (mounted on top of the cabinet).

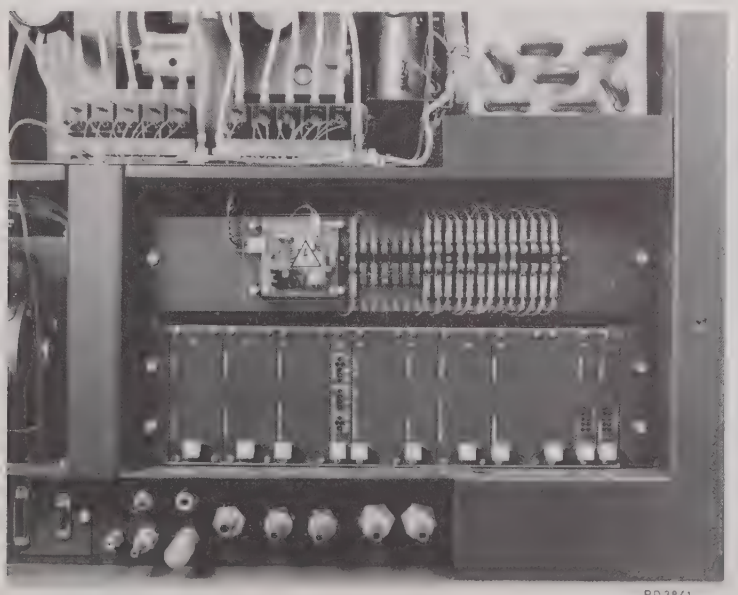


Fig. 5.1A. Rear panel

5.1.1. Manual controls

Control of the spectrometer operation is from commands given at the main terminal keyboard, but three sets of front panel push-buttons, see figures 5.1B. and C, can also be selected, as follows:

VACUUM, HELIUM, AIR — To select the atmosphere in the spectrometer chamber. A previously selected push-button must be operated to return it to the normal (OUT) position before another push-button is selected.

COUNTS, TIME, ANGLE — Interlocked push-buttons to select the function for display on the digital indicators (seven digits and decimal point).

COUNT RATE, VACUUM — Interlocked push-buttons to select the function for display on the meter — with numerical display of the full-scale reading.

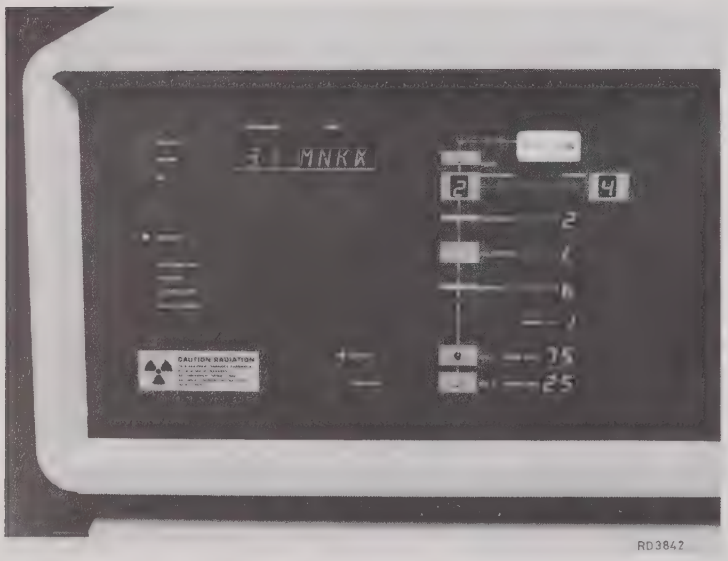


Fig. 5.1B. Front display panel

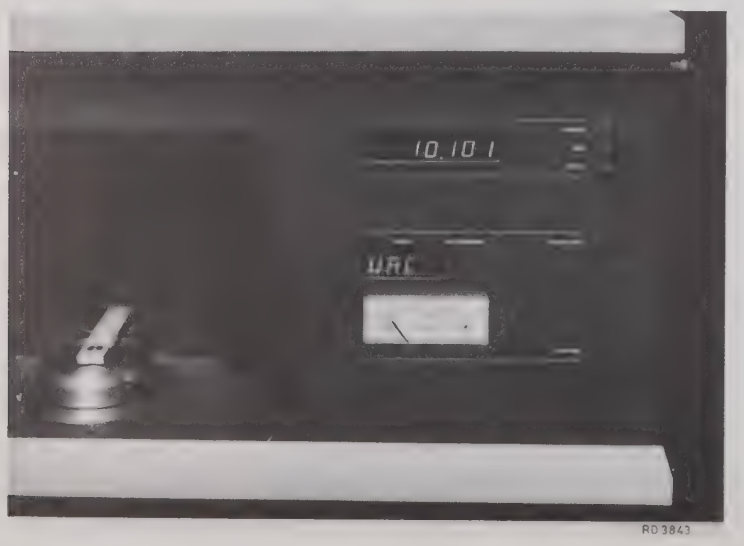


Fig. 5.1C. Front right-hand display panel

In addition to the above the following controls, etc., are situated on the right-hand side panel, see figure 5.1D.:

- Two sets of gas flow meter and gas flow adjustment.
  The left-hand set has the flow meter calibration to 3,5 litres per hour, and is part of the flow detector gas circuit. The flow is normally set between 1 and 2 l/h by adjusting the knurled knob.
  The right-hand set is calibrated to 120 litres per hour and is part of the helium gas system. The flow rate is adjusted to approximately 60 l/h.
- GAS LEAKAGE RESET; the gas flow through the flow detector is monitored, and if a gas pressure drop is detected the red (LED) warning lamp DETECTOR GAS will be lit, the solenoid valve in the gas circuit will close, any sample measurement will stop, and the message ERROR DETECTOR GAS will be printed. When the condition is corrected the reset push-button must be operated to restore normal working.
- CALIBRATE; push-button to override the scaler pulse shift correction circuit, for example when the H.T. to the gas-flow or scintillator detector is adjusted – see paragraph 6.1.
- TEMPERATURE 1 to 10; a variable control to set the stabilisation point of the temperature in the spectrometer cabinet. The range of control is approximately from 25°C to 35°C and the normal setting in a temperate climate is around the mid-position, see paragraph 1.6.5.
- C1, C2, %; three light emitting diodes to indicate the operation of the temperature stabilisation system. The proportional control circuit operates cooler 1(C1) and cooler 2 (C2), and on/off duty cycle of the heater (%) to maintain a constant cabinet temperature.
- TIME CONSTANT, AUT, .1 to 10s; the time constant of the scaler circuit output to the meter, and to a chart recorder, can be selected. If AUT is selected the time constant τ is automatically set, dependent on the selected range, where $\tau = 10^4$/range. This prevents noisy recordings.
- ATTENUATION 1, 2, 4; reduction of the amplitude of detector pulses to the amplifier and pulse height analyser circuit. Normally set to 1, but can be set to a higher value if a high level of electronic noise is experienced. In this case readjust the high-voltage to the detectors, see paragraph 6.1.
- 1500V 1x; potentiometer control from 500 to 1500 volts (1000 divisions) of the high-voltage supply to the scintillation detector, see paragraph 6.1.2.
- 3000V 2x; potentiometer control from 1000 to 3000 volts (1000 divisions x2) of the high-voltage to the gas-flow detector, see paragraph 6.1.1.

The following controls are situated on the BUS INTERFACE plug-in board (situated above the time constant control):

- BATTERY ON OFF: a battery mounted on the circuit board should be switched on to safeguard the contents of the parameter bank in the event of a power failure or disconnection of the mains power to the system (H.T. generator input).
- RESET: The operation of this push-button stops all hardware operation and the microprocessor initiation program is restarted, see page 1.4. Normal operation is possible when C = or * dialog is resumed.
- +5V
  +12V
  +5VP
  -5V
  -12V

  Five lamps (LED's) are lit to indicate correct operation of the circuit power supplies, and will extinguish if the voltage is low or zero. The power supplies are situated at the lower right-rear of the cabinet.

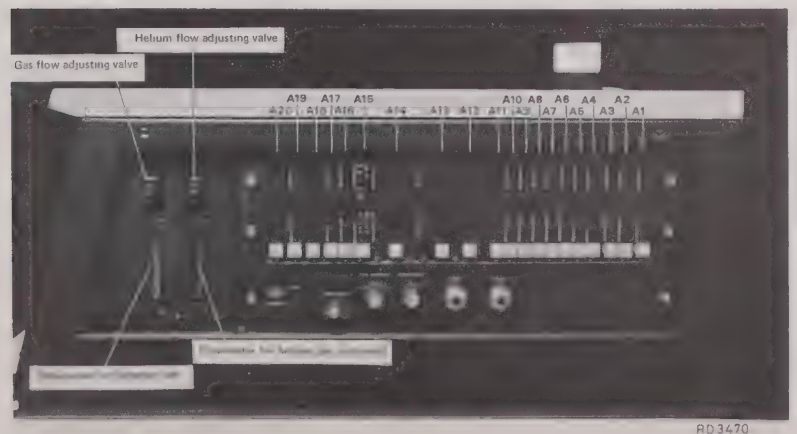


Fig. 5.1D. Side panel.

5.1.2. Front panel display

The front panel display (see figure 5.1B.) will indicate the following conditions:

- SPINNER; lit when the sample spinner is not running. (Spinner runs only during measurement.)
- DETECTOR GAS; lit when the gas flow to the flow detector is not satisfactory
- VACUUM; lit when a vacuum atmosphere is selected, but the amount of vacuum is not satisfactory
- AIR PRESSURE; lit when the pressure of the air to operate the pneumatic system is not sufficient ($< 0{,}253$ MPa = 2,5 atm), and the complete system switches off.
- SAFETY CIRCUIT; fast flash if one of the safety circuits is interrupted (to indicate a potentially dangerous situation), or a slow flash will indicate that both safety circuit loops have been interrupted. If both safety loops are correct (closed) the LED is extinguished.

The above four lamps are red LED's to indicate a fault condition.

- PROGRAM LINE; Six alpha-numeric indicators to show the measurement program list number and the element line (e.g. 09 MNKα) selected during the measurement of a sample.

The following synoptic display indicates the spectrometer conditions during sample measurement:

- X-RAYS ON; warning lamp to indicate that X-rays are being generated in the spectrometer chamber
- FILTER; lit if the beam filter is in front of the X-ray tube, i.e. FLT = Y in ACH list
- MEASURING
- LOADING

} numerical indication (1 to 4) of the turret (and sample) position.

- DIAPHRAGM; numerical indication (1 or 2) of the mask selection at the entrance collimator - see paragraph 1.6.3.
- COLLIMATOR; indication (F or C) showing fine or coarse entrance collimator selection
- CRYSTAL; numerical indication (1 to 6) of the crystal changer position. Refer to the crystal type fitted to the crystal changer positions.
- ORDER; numerical indication (1 or 2) of the order of reflection selected.
- DET 1; lit when the gas flow detector is selected
- DET 2; lit when the scintillation detector is selected
- UPPER LEVEL; two digit indication (00 to 99) of the precentage upper level setting of the pulse height discriminator.
- LOWER LEVEL; similar two digit indication (00 to 99) of the lower level setting
- SETTING; lit when the spectrometer parameters are being set, generally before the measurement of a sample.
- ANALYSING; lit during the measurement of a sample

5.1.3. Vacuum/Air system

A diagram of the vacuum/air system is shown in figure 5.1E. When the vacuum push-button is operated the vacuum pump will run, and the main vacuum valve is pneumatically operated provided that the air inlet valve and airlock inlet valve are closed. Also the airlock valve will open if the sample cap is down. The vacuum pump evacuates the spectrometer chamber and the airlock to permit sample analysis in a vacuum atmosphere.

When a sample is to be loaded the airlock valve closes and the airlock air inlet valve opens. The cap opens (with plunger high), and when the sample is loaded the cap will close before the measurement cycle commences. The air inlet valve closes and the airlock vacuum valve opens to evacuate the airlock. After a small delay the plunger goes down to allow the sample to be transported to the measuring position in the sample chamber.

When an air atmosphere is choosen the main vacuum valve is closed, and the air inlet valve opens to permit an air atmosphere in the spectrometer chamber. The airlock vacuum valve is closed and the airlock air inlet valve opens. The vacuum pump is not running.

When a helium gas system is installed the above description is modified, refer to paragraph 3.3.

The vacuum measuring system consists of two negative coefficient resistors, enclosed in epoxy resin, one in the spectrometer chamber and the other in an envelope exposed to the atmosphere. The resistors are part of a bridge circuit, arranged so that the current flowing through the meter will vary as the resistance of the sensor changes due to variation of pressure in the spectrometer chamber. The change in meter reading is not linear and is expanded at low pressures which is the area of interest. A warning lamp VACUUM on the front panel is lit until the pressure is sufficiently low. This point is adjustable and is normally set to about 30 Pa – refer to the Service Manual. Under vacuum conditions the meter reading is normally below 20 Pa (133,3 Pa = 1mm Hg, and 1 atm $\approx 10^5$ Pa).

The control circuit is on the miscellaneous control circuit board at the bottom rear of the cabinet, and a duplicate LED is lit when the vacuum is not satisfactory.
In this case an error message VACUUM ERROR will be printed before and after a sample measurement, but operation is not inhibited.

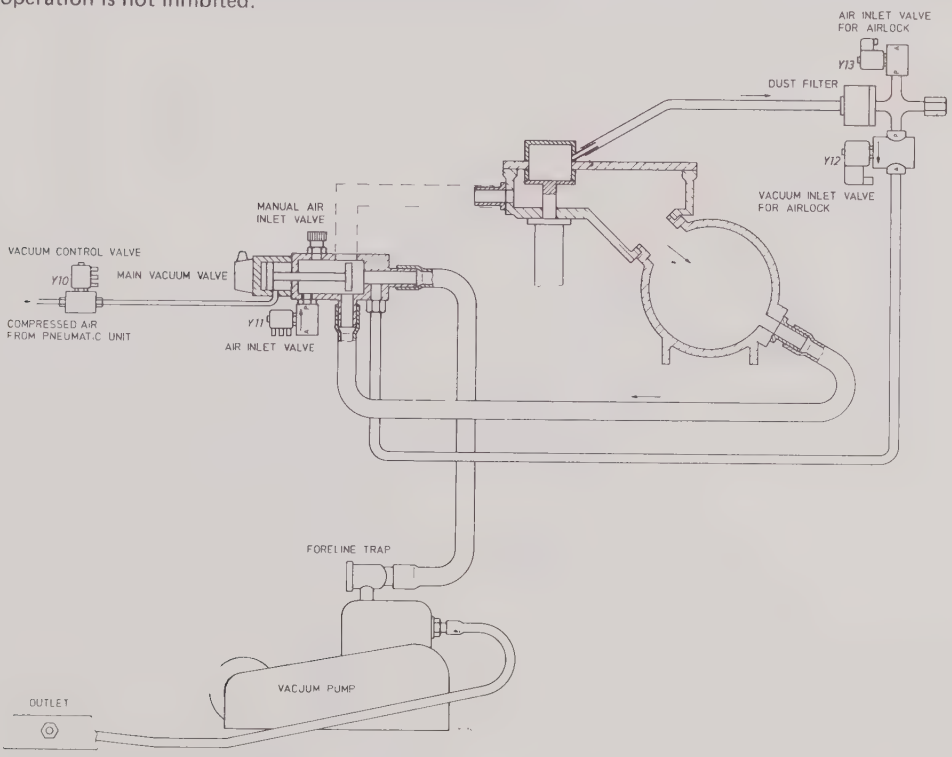


Fig. 5.1E. Vacuum/Air system

5.1.4. Temperature stabilisation system

The temperature stabilisation system maintains the spectrometer components, particularly the analysing crystal, at a constant temperature in the cabinet. A diagram of the system is shown in figure 5.1F., and includes a heater and two separate coolers, each having an electric fan. The control circuit includes an adjustable temperature control and three LED's to indicate switching of the heating and cooling elements. A very stable temperature control is possible due to the use of proportional control techniques. It is recommended that the temperature control is adjusted to maintain the cabinet to the yearly average room temperature, and readjustment of the setting must be minimal if high precision analysis is required. The range of temperature control is approximately 25 to 35°C.

One cooler is situated in the lower half of the cabinet, and the other is combined with the heater in the upper part. When the control circuit signals either of the coolers to operate, a magnetic valve opens to allow mains water to pass through the cooler radiator and a fan circulates the cabinet air through the radiator.
Note that two sets of water input and output are provided at the rear of the spectrometer cabinet, one set for the temperature control and the other set for cooling the X-ray tube and connected directly to H.T. generator water circuit.

A negative temperature coefficient resistor senses the temperature in the middle of the cabinet, and, depending on the difference between the actual and the preset temperatures, the control circuit will select one or both coolers, or the heater. The amount of heating is controlled by varying the on/off duty cycle of the heater, which is indicated by the % LED on the side panel of the spectrometer and on the miscellaneous control circuit at the rear. The operation of the coolers will be indicated by the LED's C1 and C2 on the side panel.

The variable control on the side panel will adjust the set temperature from approximately 25°C to 35°C.

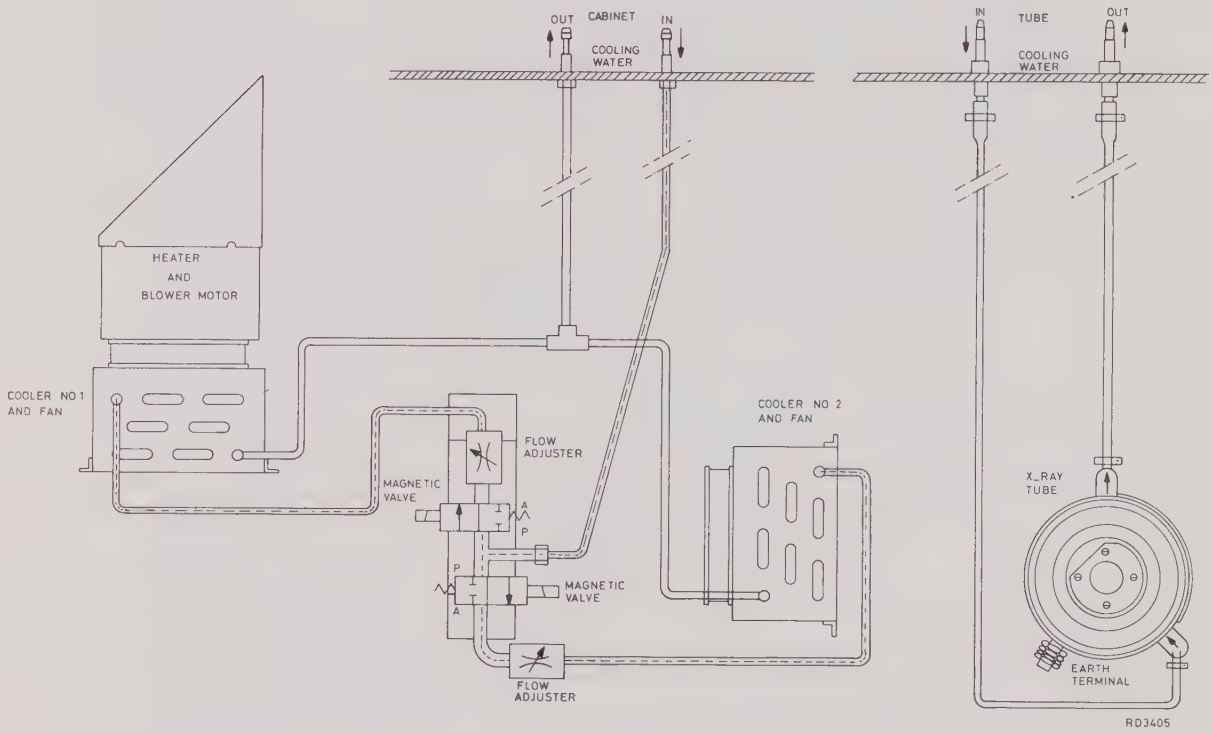


Fig. 5.1F. Cooling water circuit.

5.1.5. Counting gas system

The gas required for the gas-flow detector is a mixture of approximately 90% Argon and 10% Methane (CH_4), known as P10 gas.
The impurities in the gas may not exceed the following:

N_2	<	200ppm
O_2	<	40ppm
H_2O	<	10ppm
C_2H_4	<	250ppm
H_2	<	10ppm

The recommended gas flow rate is 1 to 2 litres per hour.

The bottle with counting gas should be placed against the wall approximately 2 metres from the spectrometer gas inlet. Before the bottle is finally installed reference should be made to the local safety regulations.

Where the gas pipe crosses the floor a wooden, metal or plastic covering should be provided for its protection.

A layout of the gas system is shown in figure 5.1G. The gas supply is connected to a gas unit, comprising a dust filter, gas pressure switch, magnetic valve, and gas density stabiliser. The magnetic valve will operate when the spectrometer is switched on, provided that the gas pressure from the bottle is sufficient to operate the gas pressure switch. If the pressure is not sufficient, possibly due to an empty bottle, the DETECTOR GAS lamp on the front panel is lit.

The gas is fed to the detector in the spectrometer chamber, via the gas leak sensor assembly mounted on the outside of the chamber just below the vacuum sensor. If the difference in the input/output flows exceeds a set limit, indicating a gas leak, the gas supply is switched off (by the magnetic valve). Also the warning lamps DETECTOR GAS on the front panel, and on the lower electrical panel at the rear, will be lit. A message ERROR DETECTOR GAS will be printed. After correcting the fault the control circuit must be reset by operating the GAS LEAKAGE RESET push-button on the side panel (auxiliary control panel).

The amount of gas flow is indicated by the flow meter on the side panel, and the gas flow is adjusted by a knurled knob at the gas outlet. The flow is normally adjusted between 1 and 2 litres per hour.

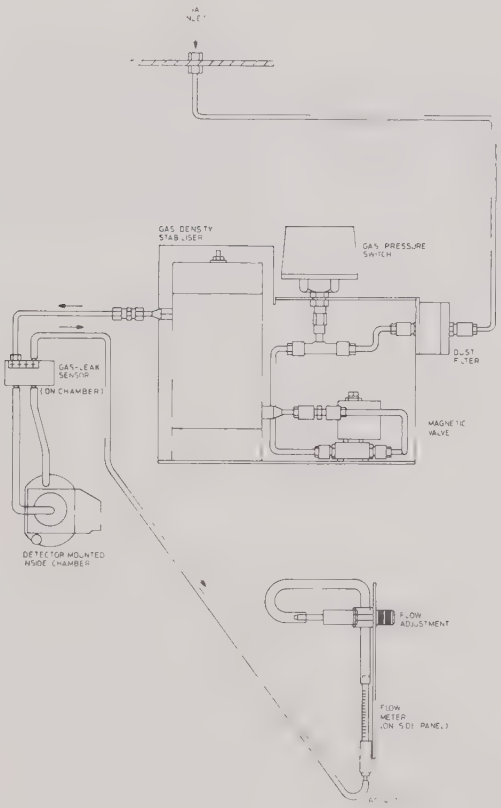


Fig. 5.1G. Detector gas system.

5.1.6. Sample handling

Samples are loaded into the spectrometer either manually, or automatically from the 6 position or 72 position sample changer. The cap and airlock are operated pneumatically, and the rotation of the sample turret is due to an electric motor. When the sample is in the measuring position an electric motor will rotate the sample (if selected) at 30 rpm (spinner) to reduce the effects of the surface roughness of the sample, and any element inhomogenity. A front panel LED is lit when the spinner is not operating.

The pneumatic system, shown in figure 5.1H., operates the following mechanical movements:

- Airlock plunger up or down
- Cap over loading position, up or down
- Filter position, in/out (front panel LED is lit when the filter is in the beam path).
- Diaphragm (mask) position 1 or 2 selection. See paragraph 1.6.3. for the mask sizes which can selected for the entrance collimator.
- Entrance collimator selection, either fine (150μm) or coarse (550μm) blade spacing.
- Main vacuum valve operation, open/closed
- PW 1505 Reference Tray option, if fitted

The cap will be raised to allow a sample to be loaded when a start measurement, load monitor, or SLP command is given. The cap can only be opened if the turret is stationary and loading position plunger is raised. This ensures that a vacuum or helium atmosphere is maintained in the spectrometer chamber during sample loading. After loading the sample the cap will come down in order to preserve the chamber atmosphere, so that the plunger can come down and the sample turret can rotate. After sample measurement the turret will rotate if more than one sample is to be measured, see paragraph 1.4.5., and the above cap/plunger movements are reversed. The chamber atmosphere is maintained at all times.

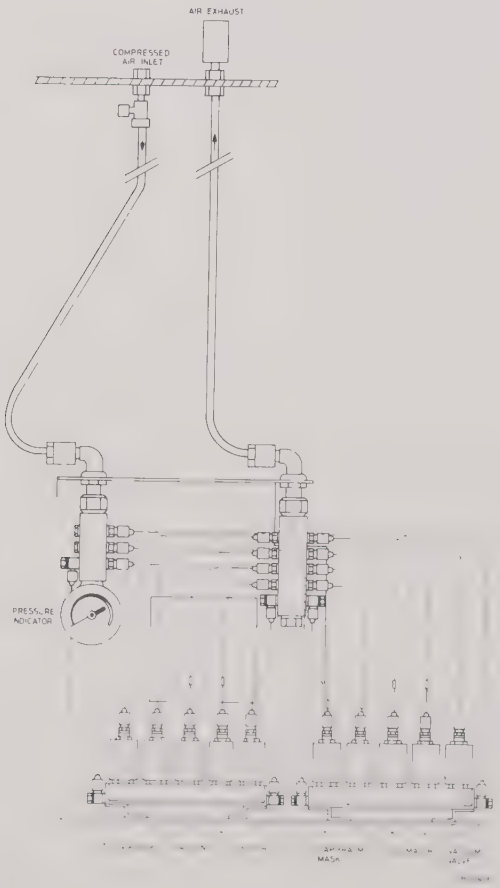


Fig. 5.1H. Pneumatic system.

5.2. DATA PROCESSOR

The data processor which can be added to the basic spectrometer unit is the P851M Minicomputer, or the Digital Equipment Corporation PDP 11/04 Minicomputer. Both systems use flexible discs to contain the software programs and to store data. A two-station disc drive unit is supplied in the PW 1790/10 Minicomputer system.

A complete set of manuals is supplied with the minicomputer, flexible disc units, and peripherals, so that a further description is not included in this paragraph, but reference regarding operation should be made to paragraph 2.1.2.

5.3. H.T. GENERATOR

The PW 1400 X-ray Spectrometer will require an H.T. supply to be connected to the X-ray tube in order to generate X-rays. A 3kW X-ray tube is installed in the spectrometer, and the tube anode material can be Cr, Rh, Mo, W, Au or Ag.

The H.T. generator PW 1732/10 or PW 1730/10 are designed for operation with the PW 1400, the cabinet design of the generators are similar to the spectrometer to allow the two units to be bolted together, with the PW 1790/10 computer if required.

The PW 1732/10 is a 100kV, 3kW unit, and will normally be dedicated for use with the spectrometer.

The PW 1730/10 is a 60kV, 4kW unit, designed to generate H.T. for simultaneous use by the spectrometer and a diffractometer when various optional units (PW 1742, PW 1743, etc.) are fitted. Although 4kW can be generated for simultaneous use, the power to the spectrometer tube is automatically limited to 3kW by the PW1400 software (see PWR command). The PW 1745 Overload protection unit can be fitted to the generator to provide additional protection, by limiting the power and kV separately to both tube systems. The spectrometer tube must be tube 1 in a simultaneous system — refer to the PW 1730 series Service Manual.

5.3.1. Front panel controls

The front panel controls of the H.T. generator are as follows:

MAINS	I	— a momentary operation of the push-button will switch on the generator and the white lamp will light. Power is applied to the PW 1400.
	O	— a momentary operation will switch off the generator.
HIGH VOLTAGE	I	— a momentary operation of the push-button will switch on the generator H.T. to the X-ray tube(s), and the white lamp and X-RAYS ON lamps will light.
	O	— a momentary operation will switch off the H.T. to the tube, but not the a.c. and low-voltage supplies.
X-RAYS ON		— warning lamp above the push-buttons to show that the tube is producing X-rays. The H.T. is automatically switched off if a bulb fails. A PW 1161 warning lamp can be mounted on top of the cabinet, or in a conspicuous position, to provide additional warning.
kV 20 - 100		— switch to manually select value of the high-voltage to the X-ray tube, in steps of 5kV. Must be in minimum position to switch on H.T.
kV meter		— meter to indicate the H.T. applied to the X-ray tube.
mA 10 - 80		— switch to manually select tube current in steps of 5mA. Must be in minimum position to switch on H.T.
CAL -5		— variable control to adjust tube current from 0 to -5mA, from the main mA switch setting.
mA meter		— meter to indicate the current through the X-ray tube.

The SHUTTERS controls, etc. are used when a tube tower for diffractometry is installed.
Push-buttons to select tube 1 or 2 operation, and the X-ray tube filament voltage (11V or 13V) are on a small rear panel (non-simultaneous use), and will rarely require any re-selection.

5.3.2. Simultaneous use with a diffractometer

The H.T. generator can be used simultaneously with a diffraction equipment, provided the combined simultaneous power requirement is less than 3kW (PW 1732/10) or 4kW (PW 1730/10).

The PW 1742 HV Switch, required when two tubes are used simultaneously or sequentially, does not have any panel controls.

The following two optional units have controls:

PW 1743 Simultaneous unit

The front panel controls are similar to those on the main control panel. The tube selection push-buttons on the PW 1730 rear panel are no longer operative, and are replaced by the TUBE 1 I and O, and TUBE 2 I and O, push-buttons on the PW 1743 front panel.

The mA switch and CAL to −5mA controls adjust the current of tube 2, which is indicated on the mA meter.

The shutter controls for a tube tower are as described in the generator manual.

The filament voltage for tube 2 is set to 11 volts, and the tube must be a diffraction tube and isolated.

PW 1745 Overload protection unit

The circuit board is plugged into the main board of the H.T. generator control chassis, and has four slide switches on the top edge, see figure 5.3A.

kW1 and kW2 — switches to select the maximum power limit of control settings for X-ray tube 1 or tube 2. Can be set to 0,9; 1,2; 1,3; 1,5; 1,8; 2,0; 2,2; 2,4; 2,7 or 3,0kW.

mA1 and mA2 — switches to select the maximum tube current control settings for X-ray tube 1 and tube 2. Can be set to 40, 50 or 60mA, or OFF.

Note: If two X-ray tubes are operated sequentially, i.e. without PW 1743, the kW2 and mA2 switches are not operative and maximum limits for **both** *tubes are set by kW1 and mA1.*

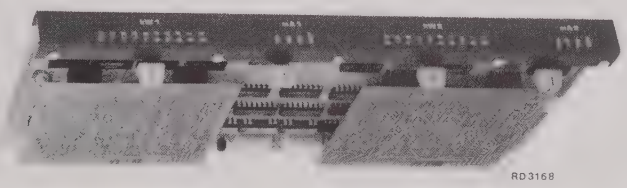


Fig. 5.3A. PW1745 Overload protection unit.

6. ALIGNMENTS AND ADJUSTMENTS

The PW 1400 system should be regularly maintained in accordance with the recommendations in the Service Manual, and having regard to local conditions and use. For example, the continual measurement of powder samples will require a greater attention to cleanliness , and more frequent replacement of the dust filter for the airlock; and the water filter in the H.T. generator may require frequent cleaning if the water supply is contaminated. The purpose of this section of the Operation Manual is to detail the alignments and adjustments which are necessary to ensure optimum performance of the spectrometer.

The system is designed for continuous operation, but even when switched off the connection to the mains supply should not be removed as the stabilisation of the cabinet temperature is then not operating, also the parameter bank contents will be lost if the internal battery is discharged, refer to paragraph 1.3.4.

WARNING

Exercise extreme care at all times if X-rays are being generated with any of the safety devices temporarily overriden during the following procedures, for example, when adjusting the crystal. Always work with the lowest possible kV and mA generator settings, and avoid any exposure to X-rays. Switch off the generator before handling any component in the X-ray beam path.

Checks and adjustments must only be performed by experienced personnel in accordance with local safety regulations.

6.1. SETTING THE DETECTOR HIGH-VOLTAGE

The setting of the two high-voltage potentiometer controls situated under the right-hand side panel is described. The potentiometers can be set from 500 to 1500, corresponding to 500 to 1500 volts for the X1 (left-hand) control and 1000 to 3000 volts for the X2 (right-hand) control. The high-voltage to the gas-flow detector is set by the X2 potentiometer (up to 3000V), and for the scintillation detector by the X1 potentiometer.

The following procedure are based in the measurement of the CuKα line in a copper sample, with manual control of the H.T. generator to give an intensity of approximately 20 000 counts per second.

Note that the CALIBRATE push-button on the side panel must be depressed when the high-voltage potentiometers are being adjusted. This action disables the automatic pulse shift correction circuit.

6.1.1. Gas-flow detector

To set the high-voltage to the gas-flow detector proceed as follows:

– Assemble, change, or check that the copper channel (ACH CU) is as below:-

NAME := CU
LINE := KA
FILT := NO
COLL := F
DET := F
XTAL := (Position for LIF 200)
ORDE := 1
% VL := 80
% LL := 20
KV,MA := 0 (manual setting)
ANGL := 45.03
-OFFSET:= 0
+OFFSET:= 0

- At the left-hand side of the front panel operate the AIR push-button (VACUUM and HELIUM normal). At the right-hand side operate the meter COUNTRATE and display COUNTS push-buttons (or ANGLE as required).
- Remove the top right-hand side panel.
  Check that the X2 potentiometer does not exceed a setting of 900 at any time, i.e. the H.T. to the gas-flow detector is 1800 volts maximum.
- Load the copper sample (SLP and SMP commands).
- Give the SCH CU command to set the channel parameters,
- Adjust the H.T. generator kV and mA control until the meter indicates approximately 20 000 counts per second. If necessary, readjust the goniometer angle to obtain the maximum countrate reading, refer to paragraph 6.5.
- Now give the commands LWL 49 and UPL 51, to set a window of 2% symmetrically at 50% lower level. Select a suitable ratemeter scale (RMS).
- Hold the CALIBRATE push-button depressed (on side panel) and adjust the X2 HV potentiometer until a maximum countrate indication is obtained. The voltage will be around 1700 volts, but **DO NOT EXCEED 1800 VOLTS.**

If required, the countrate can be indicated by a chart recorder.
Note that operation of the CALIBRATE push-button will disable the pulse shift correction circuit as this circuit must not be operational while the HT adjustment is made.

After the HT is satisfactorily adjusted, the lower level and upper level parameters of the copper channel set should be set to the normal values, see paragraph 4.3.4., if required.

6.1.2. Scintillation detector

The procedure is similar to that for setting the high-voltage of the flow detector, but now the detector selection in the channel set must be DET = S. The H.T. generator is set to produce an intensity of 20 000 cps from the Cu sample.

Follow the previous procedure, and after LWL = 49 and UPL = 51 commands are given, adjust the X1 HV potentiometer until a maximum countrate is indicated, with the CALIBRATE push-button operated. The voltage will be approximately 1000 volts, but **DO NOT EXCEED 1200 VOLTS.**

6.2. DETECTOR MAINTENANCE

Maintenance of the scintillation detector is not possible, but if the resolution for the measurement of the CuKα line in a copper sample is greater than around 50% then the measurement results will probably be affected and replacement of the scintillation tube should be considered.

As mentioned in paragraph 4.4.2., the contamination of the flow counter will cause a deterioration of the detector resolution, and if the resolution of the CuKα line from a copper sample is around 20% this may not be acceptable. In this case clean the flow counter chamber and replace the counter wire.

If the vacuum in the spectrometer chamber deteriorates it is possible that the gas-flow detector window is perforated or cracked, and the window replacement is also described.

6.2.1. Cleaning and wire replacement

When the gas flow detector requires cleaning it is not necessary to remove the complete flow detector from the crystal chamber. In practice only the ionization chamber of the flow detector need be removed, leaving the amplifier in its housing, and the mounting bracket in the crystal chamber.

The procedure is as follows:

- Bring the goniometer to 100 degrees, using the command SLF100. This places the detector in a suitable position for removal.
- Switch off (MAINS 0), and remove the cabinet front panel.
- Select air, allow time for air inlet.
- Close the gas supply, then remove the cover of the crystal chamber.
- Remove the two screws (1) and the end cap (2) leaving the gas inlet hose connected to the cap, see figure 6.2A.
- Remove the two screws (4) and the ionization chamber (3). Handle with care since the gas flow detector is close to the upper analysing crystal.

Note: Each end of the ionization chamber is sealed with an O-ring. Ensure that these rings are removed with the ionization chamber.

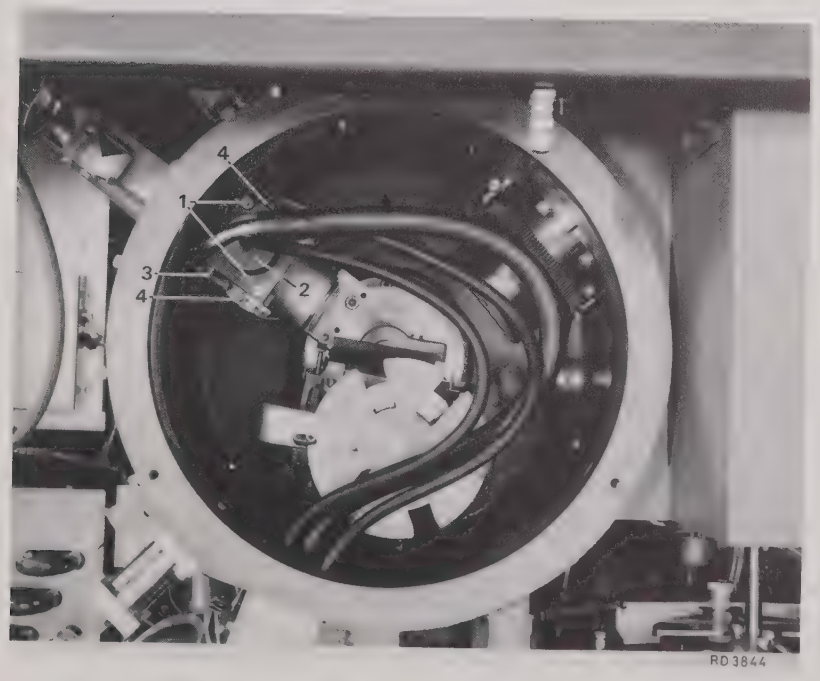


Fig. 6.2A. Crystal chamber and flow detector

To remove the detector wire, clean the chamber, and fit a new wire proceed as follows:

- Remove the flow detector collimator, the O-ring (12) and the entrance window (11) by taking out the four fixing screws, see figure 6.2B.
- Cut the tungsten wire (5), unscrew the wire holder (8) and remove the second wire holder (1).
- Tap the conical pins (9) and (13) out of the wire holders using a thin needle. If this proves difficult or if damage results, discard the holders and pins and use new ones.
- Rinse the ionization chamber and the collimator thoroughly in a bath containing clean alcohol or petroleum ether.
- Shake to remove excess cleaning fluid and leave them to dry completely. If clean compressed air is available this can be used to aid drying, particularly of the collimator.
- Cut off a piece of new 50μm diameter tungsten wire 20cm (8 inches) long. Ensure that the wire is clean and free from oxidation by cleaning with petroleum ether.
- Feed the wire through the wire holder (1) so that it protrudes approximately 2cm (0,75 inch). Wedge the wire in the holder by tapping in the conical pin (9).
- Feed the wire through the insulators (2) and (7) using tweezers or a thin needle. Press the holder (1) into the insulator (2).
- Feed the wire through the holder (8) and screw the holder into the insulator (7) until it is in the centre of the treaded portion. Make sure that the holder (1) is pressed fully into the insulator (2) and that the insulators (2) and (7) are properly located.
- Pull the wire taught and wedge the wire in the holder (7) by tapping in the conical pin (13).
- Slightly stretch the wire by rotating the holder (8) in a counterclockwise direction.

CAUTION **Avoid overstraining the wire. The amount by which the holder (8) must be rotated depends on the original taughtness of the wire and care is necessary.**

- Trim off the excess wire so that the protruding ends are flush with the conical pins at both ends.
- Again rinse the ionization chamber in a bath containing clean alcohol and check that the vacuum surfaces and O-rings are clean and intact.
- Place a new entrance window (11) on the ionization chamber. This window is of plastic foil with a copper mask on one side. Place the mask so that the copper side faces the wire and the foil side faces the collimator.
- Fit the O-ring (12) and screw the collimator to the ionization chamber with the four fixing screws. Ensure that the collimator is fitted with the bevelled edge at the top.

To replace the flow detector

- Check that the contact spring (10) and the O-rings (3) are in position and screw the ionization chamber to the amplifier housing.
- Place the O-ring (6) in position and screw the end cap on the flow detector.
- Check the resolution of the flow detector as previously described in paragraph 4.4.3.

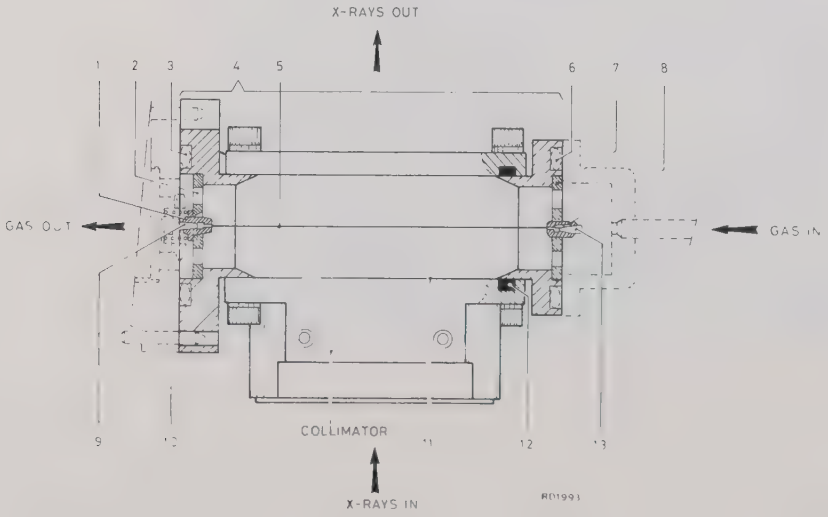


Fig. 6.2B Flow detector ionization chamber

6.2.2. Replacing the detector entrance window

The entrance window permits low energy radiation to pass into the gas flow detector with a minimum loss by absorption. Because the pressure within the flow detector is approximately one atmosphere and that in the crystal chamber surrounding the flow detector is frequently evacuated, it is probable that after some time the window will be perforated or cracked. A faulty entrance window will be indicated by:

1. A loss of vacuum, i.e. the reading on the vacuum meter (the two front-panel VACUUM push-buttons are operated) will not reach the normal low value.
2. Higher gas consumption resulting in a lower gas flowmeter reading.
3. In some cases a loss in pulse height revolution.

As the gas leakage increases an error message "ERROR DETECTOR GAS" will be printed during sample measurement. The front panel "DETECTOR GAS" lamp will be lit, and the measurement is inhibited.
After the window is replaced the side panel GAS LEAKAGE RESET push-button must be operated before normal operation is possible.
In the event that the vacuum leakage increases, a warning "ERROR VACUUM" is printed, the front panel warning lamp VACUUM is lit, but operation is not inhibited.
The procedure for replacing the flow detector entrance window is similar to that described in paragraph 6.2.1. However, it is recommended that the whole flow detector with its mounting bracket be removed from the crystal chamber, although with care only the collimator, O-ring, and window need be removed. In either case it is not necessary to remove the flow detector end cap.

- Check the O-ring and vacuum surfaces for damage and cleanliness and the collimator for dust particles and damage to the blades.
- Clean the collimator in a bath containing petroleum ether, if necessary.
- Reassemble the collimator, O-ring, and new entrance window (copper mask facing the detector wire and foil facing the collimator).
- Carefully replace the flow detector in the crystal chamber, and replace all covers, etc.
- Operate the generator MAINS 1 push-button, and then the generator "GAS LEAKAGE RESET" push-button.

Note: **The flow detector bracket is positioned on two dowel pins. These pins are a tight fit in the bracket, so it is essential to ensure that the fixing screws are fully tightened and that the bracket is properly seated on the mounting ring.**

6.2.3. Changing the gas cylinder

The detector gas system comprises a gas cylinder fitted with a gas reduction valve, supplying gas to the spectrometer through tubing. A gas density stabilizer, dust filter, gas flowmeter and gas flow adjusting valve are mounted in the spectrometer and are described in the Service Manual.
An empty gas cylinder will operate the gas pressure switch and sample measurement is inhibited. The DETECTOR GAS lamp will be lit.

Detector Gas

The specification for the argon/methane gas used in the gas flow detector is as follows:

Type		: P10
Volume per cent	Ar	: 89 - 91%
	CH_4	: 9 - 11%
Impurities	N_2	: $<$ 200 ppm
	O_2	: $<$ 40 ppm
	H_2O	: $<$ 10 ppm
	H_2	: $<$ 10 ppm
	C_2H_4	: $<$ 250 ppm

This procedure involves the use of gas at high pressure. Follow the procedure carefully to ensure that the window of the gas flow detector is not ruptured when the gas pressure is reapplied.

To change the gas cylinder proceed as follows:-

- At the spectrometer, release button "VACUUM" and select AIR.
- At the gas bottle reduction valve turn the output adjuster fully counterclockwise, thus reducing the output pressure.
- Firmly close the main valve on the cylinder, turning it clockwise.
- Remove the reduction valve assembly from the cylinder by unscrewing the coupling nut. The coupling nut which attaches the reduction valve to the cylinder has a left-hand thread. Turn it clockwise to slacken it and counterclockwise to tighten it.
- Replace the protective nut on the cylinder output connection and fit the domed cover.
- Renew the gas cylinder, and ensure that the new cylinder is securely positioned. Remove the protective domed cover and the protective nut on the output connection.

Warning: **Gas cylinders are dangerous if not handled with care.**
Always follow the local safety regulations.

- Before fitting the reduction valve assembly fit a new Teflon washer inside the coupling nut and ensure that the cylinder is at room temperature.
- Any dust particles in the cylinder connection can be blown out by quickly opening and closing the main valve, ensuring that the cylinder output connection is pointed in a safe direction.
- Fit the reduction valve assembly by screwing the coupling nut in a counterclockwise direction. Ensure that the feed pipe does not turn by gripping the pipe with a suitable tool.
- Check that the supply connection to the spectrometer is correctly made.
- Open the main valve on the cylinder and check that the cylinder pressure gauge registers approximately 150 kgf/cm^2.
- Rotate the output adjuster slowly and carefully in a clockwise direction until the output pressure gauge registers 0,7 atm.
- If desired the joints can now be checked for leaks with a soap solution. If this is done make sure that all soap is thoroughly washed off with clean water afterwards to ensure that no soap can enter the system when the joints are subsequently opened.
- Open the gas flow adjusting valve fully for several seconds to flush the system and then close it until the flowmeter indicates 1 litre/hour.
- Select a VACUUM atmosphere
- When all the air is flushed out of the system check the quality of the detector gas.
  A difference in the gas composition can shift the value of the pulse height setting from its normal working value of 50% and this can be corrected by resetting the value of the detector high-voltage as described in paragraph 6.1.1.
- Operate the GAS LEAKAGE RESET push-button in order to resume sample measurement-operation.

High Pressure Gas Leakage Check

This procedure should be employed each time a cylinder of gas is connected to the spectrometer to ensure that there is no leakage of gas on the high pressure side of the reduction valve.
It is better not to use a soap solution test because it would be possible for dried soap to enter and contaminate the system when the cylinder is subsequently changed.
If such a test is used all soap solution must be carefully washed off when the test is concluded.

- Close the reduction valve fully. In this condition the output adjuster will be turned fully counterclockwise.
- Open the main valve slowly. The cylinder pressure gauge will record a value of approximately 150 kgf/cm^2. Make a record of the pressure reading.
- Close the main valve of the cylinder fully and leave in this condition for approximately 30 minutes.
- At the end of this period compare the pressure reading with the pressure previously recorded.
  If the pressure is unchanged, there is no leak present. If the pressure has dropped this indicates a leak in the high pressure connection. Open the output adjuster slowly to release any residual pressure and then fully close it again. Disconnect the cylinder, clean the coupling carefully with petroleum ether, reconnect the cylinder and repeat the high pressure gas leakage check.

6.2.4. Gas Density Stabilizer Check

The following procedure may be used to check the correct operation of the gas density stabilizer:

- Close the output adjuster until the output pressure gauge indicates approximately 0,3 atm.
- Adjust the gas flow until the flowmeter indicates 1 litre/hour.
- Open the output pressure adjuster slowly until the output pressure gauge indicates approximately 1,2 atm.
- Check that the indicated flow rate has not changed by more than a small amount.
  This pressure increase by a factor of four should cause very little increase in the flowrate if the gas density stabilizer is operating correctly. If the flowrate increases significantly it is probable that the gas density stabilizer required cleaning. This can only be done by an experienced service engineer.
- Slowly reduce the output pressure to 0,7 atm.

6.3. ANALYSING CRYSTAL

Up to six analysing crystals can be fitted on the crystal changer, which is mounted in the spectrometer chamber. The crystals can be selected from the following types:

PW 1530/30 - LiF 200 crystal
PW 1532/30 - ADP crystal
PW 1533/30 - EDDT crystal
PW 1535/30 - PE crystal
PW 1536/30 - KAP crystal
PW 1538/30 - LiF 220 crystal
PW 1591/30 - Ge crystal
PW 1592/30 - TlAP crystal
PW 1593/30 - Graphite crystal
PW 1594/40 - InSb crystal

Most crystals are hygroscopic and should be stored in a vacuum, or in a hermetically sealed cointainer with some desiccant (silica gel, etc.) inside. Crystals are delicate and must be handled with care, for example, a TlAP crystal may crack if subjected to a change in temperature, **DO NOT TOUCH THE SURFACE** but hold at the edges only. TlAP is toxic and this crystal must be handled with gloves.

6.3.1. Alignment

Crystal alignment is not normally necessary, but should be carried out after crystal replacement or if measurement results suggest that realignment is necessary. This should be done when the cabinet temperature is stabilised.

The following items are supplied with the spectrometer to be used for crystal alignment:

- Plastic cover to replace the spectrometer chamber front cover.
- Adjusting screwdriver.
- Cover microswitch operation assembly - two brass bars (2½ cm long) with two coiled springs.

Follow the procedure below and carefully observe all cautions, particularly when X-rays are being generated:-

- Switch off the HT generator/spectrometer, after setting the kV and mA controls to minimum.
- Remove the front cover of the spectrometer cabinet, and override the cover safety switch. Ensure the safety switches are returned to the normal position after crystal alignment is complete.
- Remove the front cover (and drive motor) from the crystal chamber.
- Fit the cover microswitch operation assembly, so that the microswitch is operated by the supplied assembly

- Operate the generator MAINS I push-button.
- Assemble a channel set, or change an existing set, to suit the crystal to be aligned, according to table 6.3A.

Table 6.3A. — Conditions for crystal alignment

Crystal	*Sample*	*Element*	*Vacuum*	*2θ angle*
LiF 220	Cu	Cu	N	65.56
LiF 200	Cu	Cu	N	45.03
Ge	NaCl	Cl	Y	92.76
	or S (2)	S	Y	110.69
Graphite	NaCl (1)	Cl	Y	89.53
	or S (2)	S	Y	106.29
InSb	Si (3)	Si	Y	144.76
PET	Al	Al	Y	145.13
ADP	Mg (4)	Mg	Y	136.67
TlAP	Al	Al	Y	37.80
	or NaCl(1)	Na	Y	55.10

Notes 1. **Press NaCl (table salt) into a solid pellet, e.g. at 20 tons for 30 seconds.**

2. **Sample should have a high sulphur content, but be essentially free of molybdeum e.g. pure sulphur .**

3. **A high silicon sample e.g. PW 1302/00, or pure chemicals or a geological sample e.g. granite, or ferrosilicon.**

4. **High magnesium sample e.g. solid pellet of MgO, or high magnesium alloy.**

All other spectrometer conditions to be as the table in paragraph 1.3.1. (FLT, COL, DET, ORD, UPL and LWL), except that kV and mA must be manually controlled (= 0).

- Load the sample, using the SLP and SMP commands.
- Give the set channel command (SCH CU for example).
- Switch the H.T. on (generator HIGH VOLTAGE I push-button), and adjust the kV and mA controls to give a sufficient intensity.
- Observe the intensity, either by the deflection of chart recorder (give RMS command), and /or using the countrate meter (COUNT RATE push-button depressed), or by using a job list to obtain a digital read-out - give AJB xx, SCT EJB, plus PTS 10 (10 seconds count), RCJ0 (continuous recycle) and SJB.
- Place the plastic cover over the spectrometer chamber, with the adjusting screwdriver inserted to engage the crystal position adjustment screw, see figure 6.3A.
  Hold the cover in place.
- Select vacuum, as table 6.3A., by operating the VACUUM push-button. First release the AIR push-button.
- Adjust the crystal for a maximum intensity reading.

Important: **Be most careful that no part of the hand or body is in the spectrometer chamber when X-rays are present. Switch off the H.T. as soon as possible.**

- Select an air atmosphere and remove the adjusting screwdriver before selecting another element channel to be used for other crystal alignment, i.e. before any mechanical movement of the crystal changer and detector.
- Select an air atmosphere when all alignment is complete, switch off the H.T. and MAINS, remove the plastic cover and microswitch operation assembly, and fit the spectrometer chamber cover and the cabinet front panel (after releasing the safety microswitch.)

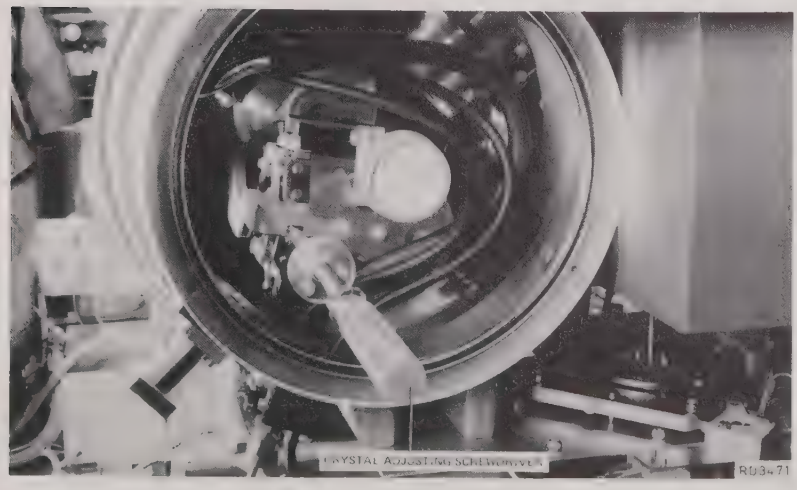


Fig. 6.3A.

6.3.2. Replacement

To replace a crystal, by a new or different type, follow the procedure below:

- Switch off, and remove the cabinet front cover and the chamber cover — see paragraph 6.3.1.
- Slide out the old crystal from the changer, and replace with the new crystal. Ensure the crystal is central and will not jam during rotation of the changer. **DO NOT TOUCH THE SURFACE OF THE CRYSTAL,** hold at the edge, and use gloves with the TIAP crystal.
- Replace the chamber cover and the cabinet front panel cover (for temperature stabilisation)
- If the changer position was previously empty, or has been replaced by a different crystal type, the jumper settings of the SPECTROMETER CONTROL 1 circuit board, fitted at the right-hand side panel, must be set. A shorting plug must be set to select a correct resistor, and for the main crystal types these values are already fitted. Two spare sets of jumper connections can be used for the unusual crystal types, and the resistor value will differ — refer to the Service Manual.
- Align the crystal after temperature stabilisation, if required — see paragraph 6.3.1.

6.3.3. Cleaning

Analysing crystals will not normally require cleaning, in fact any such handling should be avoided. In the event of a mishap when powder or liquid may find its way into the chamber, the following procedures can be tried:

- A light powder deposit can be removed by light brushing with a soft clean brush.
- More persistant contamination can possibly be removed by placing a lint free cloth, dampened with water, on a flat surface, and draw the crystal across the cloth a few times.
- For heavy and greasy contamination the cloth can be dampened with a little solvent, such as:
  Trichlorethylene for LiF 200, LiF 220 and Ge.
  Petroleum ether for PE, TIAP, KAP and RAP.
  Do not use liquids for graphite.

Successful operation after cleaning a crystal cannot be guaranteed.

6.4. CALIBRATING A CHANNEL PEAK ANGLE

Occassionally it will be necessary to calibrate the 2θ angle of an element peak, and to ensure that the angle entered in the channel set is correct. For example, calibration of peak angles may be necessary if a crystal has been re-aligned, and the 2θ angle found will often be slightly different from the value shown in the "X-ray wavelengths and two-theta tables".

The calibrate angle routine is described in paragraph 1.4.10., which is initiated by the command CAN xxi, where xxi is the channel name. The channel parameters will determine the crystal type to be used, and the information given in table 6.3A. show the type of sample to be used for the angle calibration. Ensure that the kV and mA values chosen will produce sufficient intensity from the sample to give the required counting statistical accuracy.

In most cases the goniometer will be positioned at the 2θ angle value given from a two-theta table, and after the CAN routine the NEW ANGLE should be close to this angle — see figure 1.4Q. A wide difference in the 2θ angles will indicate that an accurate crystal alignment is necessary, and this will affect all channel 2θ angles stored in the channel sets in the parameter bank which use that crystal.

6.5. THE X-RAY TUBE

The following types of X-ray tube can be fitted in the spectrometer:

PW 2181/00	Au	anode
PW 2182/00	Rh	anode
PW 2184/00	Mo	anode
PW 2187/00	W	anode
PW 2188/00	Cr	anode
PW 2189/00	Ag	anode

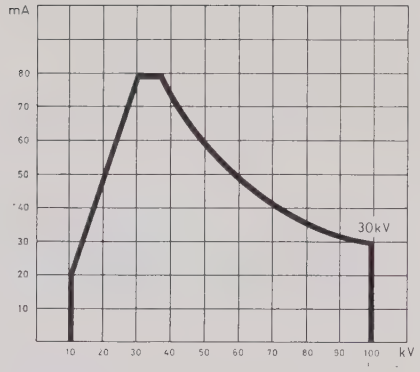


Figure 6.5B

The tubes are rated at 100kV, 3kW maximum, therefore, the manual or computer controlled settings of the H.T. generator must not exceed 3kW, i.e. kV times mA must not be greater than 3000. The maximum generator settings are illustrated in figure 6.5B.
The values of kV and mA to be input for the channel parameter sets (ACH) are indicated in the table in paragraph 1.3.1., but note that they are typical only and have been selected to give good excitation using the chromium tube. Values are indicated for a 100kV H.T. generator, and optional values for a 60kV generator are indicated in the text.

6.5.1. Care of the X-ray tube

Observe the following notes to prevent flash-over in the X-ray tube and to maximise the life expectancy of the tube. They only apply to the tubes used with the PW 1730 family of H.T. generators, and greater care may be necessary for a tube supplied from other types of H.T. generator.
If the tube has not been used for up to 100 hours, i.e. H.T. has not been applied, power up to 3kW and H.T. to 100kV can be applied immediately. However, it is good practice to apply power in steps to the tube.

If the tube has not been used for a period between 100 hours and 2 months, the generator should be set to 60kV and 50mA for a period of 5 minutes after H.T. is switched on, and before higher kV values are selected.

If the tube has not been used for over 2 months, or it is new, the high-voltage and current should be applied gradually. At switch on the H.T. generator controls are advanced to 60kV and 50mA (100kV generator). After 5 minutes set the controls to 60kV and 30mA, and then the kV control can be advanced in steps of 5kV, allowing 1 minute per step. If the mA meter shows any sign of instability (needle flickers) decrease the kV setting immediately by 5kV or more for a least a minute, then the kV control can be advanced again up to 100kV or the required value.

After the above "running in" procedures the X-ray tube is ready for normal operation

6.5.2. Changing the X-ray tube

To exchange the X-ray tube for one with another anode material, or if the tube is faulty, proceed as follows:

– Switch off the H.T. generator/spectrometer, using the MAINS 0 push-button.

The magnetic water valve in the tube cooling system will close, and the mains water supply to the system must be switched off. Do not stop the water flow by means of the manually operated tap in the H.T. generator. Note that water flow to the spectrometer cabinet temperature stabilisation system is also closed off, therefore, try to minimise the period for the following operations:

– Remove the upper rear cover of the spectrometer cabinet.

– Remove the H.T. cable clamp on the rear frame member.

– Remove the four screws securing the H.T. cable to the X-ray tube. **Allow a minimum period of two minutes from switching off the H.T. up to withdrawing the cable connector,** to allow the voltage to decay.

– Withdraw the H.T. cable connection from the X-ray tube, which may require a little force to be applied. As a precaution, touch the centre contact of the connector onto a spectrometer earth.

– Remove the safety plug (attached to a chain on the H.T. cable) from the cradle socket. Also remove the earth wire attached to the connection at the rear of the X-ray tube.

- Remove the tube clamp fixing screw, and swing the top clamp to one side.
- Carefully extract the X-ray tube from the spectrometer chamber — take care not to touch or damage the beryllium window, see figure 6.5A.
- Rest the tube on the clamp cradle, and arrange a tray or cloths to capture surplus water when the hoses are disconnected.
- Disconnect the inlet and outlet water hoses from the X-ray tube, and note the positions of the respective hoses.
- Remove the X-ray tube, and recover the O-ring.

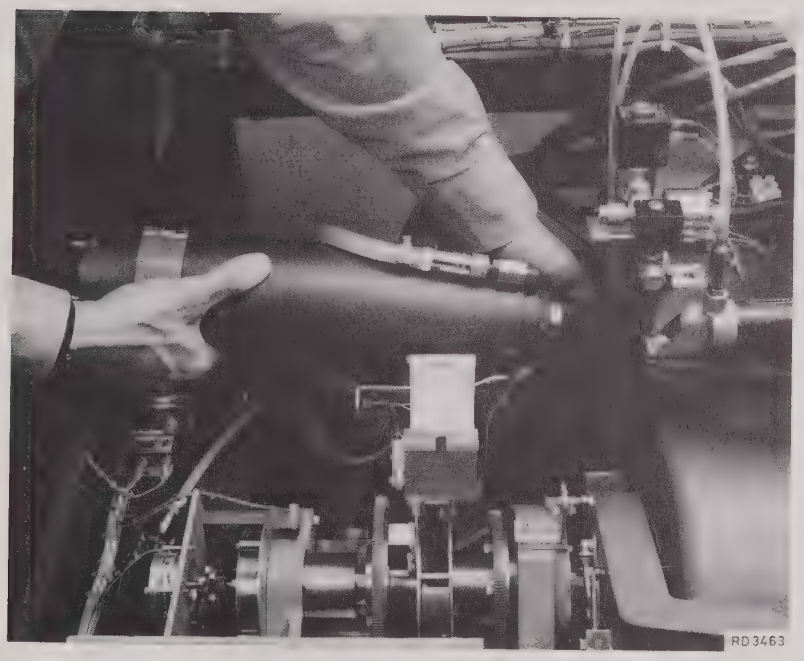


Fig. 6.5A.

Ensure that the surfaces at the chamber entrance, and the vacuum surface of the new X-ray tube, are clean and undamaged. If necessary, wipe the surfaces with a clean cloth dampened with petroleum ether.

Check the condition of the O-ring, and replace if necessary. Lightly smear the O-ring with vacuum grease (Apiezon L), and fit it on the new X-ray tube.

- Place the new tube in position on the clamp cradle.
  DO NOT TOUCH THE X-RAY TUBE WINDOW
- Connect the water hoses to the X-ray tube, and ensure that the direction of water flow is correct.
- Carefully insert the X-ray tube into the spectrometer chamber, lifting the connector end slightly to ensure that the filter mechanism or tube window is not damaged, see figure 6.5A.
  The horizontal and axial alignment of the tube should be correct, and ensure that the outlet water hose fits in the inverted 'U'-shaped guide. Push the tube fully home to make a good vacuum seal, and rotate the tube fully clockwise up to the end stop.
  Check that the safety microswitch below the tube is operated, and be careful not to damage its operating lever during the above procedure.
- Swing back the cradle clamp, and tighten the fixing screw.
- Connect the flexible earth wire to the X-ray tube earth screw, and insert the safety plug into the socket below the tube cradle.

- Coat the rubber portion of the H.T. cable connector with silicone grease, and insert it into the X-ray tube. Tighten the four fixing screws.
- Secure the H.T. cable by means of the clamp on the rear frame member.
- Replace the cabinet top rear cover, and switch on the mains supply (H.T. generator MAINS I push-button).
- Turn on the mains water supply tap, but note that water flow through the tube is controlled by the generator magnetic valve.
- Flush any air from the water hose and X-ray tube by simultaneously pressing the HIGH VOLTAGE I and 0 push-buttons for a few seconds. Damage to the tube can result if H.T. is applied before the water supply is correct. The kV and mA controls of the generator must be in their minimum positions before H.T. is switched on.
- Release the HIGH VOLTAGE 0 push-button, or operate the I push-button again, to generate H.T. to the X-ray tube.
- If the X-ray tube is new, or has not been used for a period, observe the procedures described in paragraph 6.5.1., i.e. apply kV and mA gradually. At switch on the generator is set to 60kV and 50mA (100kV generator), for five minutes. Then set to 60kV and 30mA, and advance the kV control in steps of 5kV, allowing 1 minute per step, up to the desired value.

The system is now ready for normal operation.

APPENDIX A2

1. DEC PDP11 COMPUTER OPERATION

The basic PW 1400 Spectrometer can be connected with a Digital Equipment Corporation PDP11/04 Computer instead of the Philips P851 system. When the PDP11 is used the operations described in paragraph 2 are slightly amended, and the pages peculiar to the P851 must be removed and replaced by the following pages in this appendix. A listing of the pages affected is given below.

The general description of the X-14 software package as given in chapter 2 applies for PW 1400/DEC systems and the main differences in the operation are summarised as follows:

1. The computer hardware is different and the control panel is operated differently. Therefore, the figures and description given in 2.1.2. do not apply (except for selection of input and output peripherals). Refer also to the RT-11 manual.
2. The software package is supplied on two discs, but only one need be used for assembly, analysis, regression and update. The software organisation description is changed, and the solid dots ● shown in the command listing in paragraph 2.2. are not meaningful.
3. The DEC terminology uses blocks rather than granules, therefore the description at the end of 2.1.1. does not apply.
4. Copying of disc files, initiation of a disc, and printing a disc directory are performed by the RT-11 monitor rather than X-14 software. Therefore, the commands CPF, CPD, IND and PRD are not available. For a description of these functions refer to chapter 2.7.
5. The files identification uses a six character file name plus a three character file name extension. Therefore, the file identification format as used throughout chapter 2 does not apply. For example the regression file for steel analysis is identified as STEELS.R50 rather than STLR50.
6. The empty databank on the system disc has been identified as PW 1400.DBK rather than XR14DB.
7. The designation of the flexible disc station follows the format of RT-11 software, thus the format is DX1: FILE IDENTIFICATION rather than FILE IDENTIFICATION,1. Therefore, the disc station designation as used throughout chapter 2 does not apply. For example the regression file is designated as DX1: STEELS.R50 rather than STLR50,1.
8. The format of the date as appearing in the printout is different.
9. The list of system commands (microprocessor plus computer) has been modified to show the few commands (marked with a P) which are in the P851 software, but not the PDP11 software, because similar commands are used in the dot mode, see paragraph 2.1.2.

Note that some of the X14 software (P851) readouts in paragraph 2 have not been replaced where it is thought that the file identification, date, time, output or command input format will not be confusing compared with the X14D formats.

Modify paragraph 2 of the Operation Manual, as follows:

Remove pages 2.1 to 2.8, 2.12, 2.13, 2.16, 2.17, 2.19, 2.47 to 2.51, 2.55, 2.56, 2.57, 2.60, 2.69 to 2.71, 2.75 to 2.77, 2.88, 2.92, 2.93, 2.107 to 2.109.

Insert the following pages as appropriate.

2. DATA PROCESSING

The output data from the basic (microprocessor controlled) version of the PW 1400 will show accumulated counts and measurement time for each element in the sample measuring program(s). This section of the manual will describe the X14 software and the operations possible using the intensity/time data, when a P851 computer is installed. Using these procedures an output showing the chemical concentration of the elements in samples is possible.

The operation and description of optional items, such as sample changers, helium flushing system, etc., are shown in paragraph 3.

Details of the software package developed for the D.E.C. PDP11 computer systems will be given in the Appendix of this manual.

A PW 1400/00 Spectrometer supplied with a PW 1790/10 Minicomputer system, will comprise:

- The PW 1400 Spectrometer with microprocessor and software programs in PROMs (programmable read only memories), and parameter bank capacity in RAMs (random access memories).
- A Philips P851M, connected via the PW 1400 input/output interface.
- A P830 flexible (floppy) disc unit with two stations (drive units)
- Two flexible (floppy) discs with the X14 software programs.
- One or more peripheral devices (see paragraph 3.4) with the main terminal capable of typing command information and reading out analysis data (normally hard copy). The main terminal is connected to the P851M.

2.1. DESCRIPTION OF THE SOFTWARE PACKAGE

The X14 software program to be used is on a flexible disc, normally loaded into the left-hand station (labelled 0) of the two disc drive units. A "files" disc containing measurement results and other data is loaded in the right-hand station (labelled 1).

Software notes

Sample analysis will use the microprocessor software described in paragraph 1, in addition to the computer software described in this paragraph. Therefore, the operation notes on pages 1.3 to 1.5 should be studied in conjunction with these notes before using the spectrometer system.

Copy the delivered X14 software programs onto flexible discs (for daily use), and keep the system (master) discs in a safe place - refer to paragraph 2.7.2.

Commands used in the X14 software are similar to the microprocessor commands, and the comments at the start of paragraph 1-2 will apply, e.g. commands are three letter abbreviations, etc.

Correction of a letter, or a line of input, is possible provided that a carriage return has not been given, refer to page 1.5.

Databank and parameter banks

Parameter bank is the name given to the information contained in the **microprocessor** memory (RAM), and consists of channel sets (CH), measurement program lists (MP), and job lists (JB), see the microprocessor description in paragraph 1. It is used for spectrometer control. Keyword: spectrometer operation.

Databank is the name given to the information contained in the **minicomputer** memory, and consists of link programs (LP), countrate correction sets (RC), calculation parameters (CP), monitor buffer list (MB), moduli list (ML), moduli sets (MS), names list (NM), and limits list (LL). It is used in the data handling. Keyword: Calculations (and results reporting).

Databank assembly

One of the two system discs delivered is intended for routine operation – the AN disc with the assembly, analysis, and hardware test modules. It also contains a databank designated XR14DB, which is automatically loaded when the system is started and initiated, see paragraph 2.1.2. The parameters which are input by the X14 software (ALP, ARC, ACP, etc.) go to the computer and are immediately stored in the disc databank. This disc has space for parameters loaded by the microprocessor software, i.e. the parameter bank.
If required, a files disc can be used to contain databanks and parameter banks, as follows:

Place an initiated flexible disc (see paragraph 2.1.2.) in disc drive 1 and give the command WDB xxxx, 1 which copies the empty databank XR14DB to the files disc under the name xxxx. Now load that databank again to the memory, using the command LDB xxxx, 1. All future list assembly will now be stored in the databank file xxxx in the files disc in disc drive 1, until another file is loaded. The PMM command can be given to show which databank has been loaded, and to readout details of its contents.

Writing and loading of databanks

Databank files are identified with a four character identification, plus a file type identification (the letters DB). The file type identification is automatically added when the WDB and LDB commands are given, so a databank can be loaded from a disc using the command LDB xxxx, where xxxx is the identification name of the databank file.

The PMM command will give a readout of the databank name, and the contents of the loaded databank.

The loaded databank can be written to disc, that is copied, using the command WDB xxxx, where xxxx is the identification name on the disc for the databank file, e.g. LAST (for low alloy steels). If a databank file with that name already exists on the disc, the file is overwritten with the input data and this enables the updating of databank files.

The WDB and LDB commands are executed on the disc loaded in station 0 (system disc), unless otherwise specified, i.e. the default value is 0. If the disc in station 1 has to be used, it is selected by adding a comma (or space) and 1 as a command argument, e.g. LDB xxxx, 1 or WDB xxxx, 1.

Parameter banks

The assembly of parameter bank information (ACH, AMP, AJB) proceeds directly with the microprocessor, and data are stored in a RAM. Hence, the input data are not written automatically to disc, but the complete parameter bank can be written to disc by the operators command DPB. This command causes the whole contents of the parameter bank to be written to the disc into a parameter bank file. An identification name for this file is not specified when the DPB command is given, and the parameter bank data will be written to a file on the disc from which the databank is loaded, and will have the same file name identification as the databank identification. The parameter bank data will have a file type identification PB to distinguish it from the databank data.

A parameter bank file can be read into the RAM again, using the RPB command, after loading the corresponding databank (which has the same name as the parameter bank data).

Files identification

Databank	— 4 characters, plus DB	(file type identification)	e.g.	LASTDB
Parameter bank	— 4 characters, plus PB	(file type identification)	e.g.	LASTPB
Concentrations file	— 3 characters, plus Cxx	(file type identification)	e.g.	STLC50
Regression file	— 3 characters, plus Rxx	(file type identification)	e.g.	STLR50
Recalibration file	— 3 characters, plus Bxx	(file type identification)	e.g.	STLB50
Job file	— 3 characters, plus yyz	(file type identification)	e.g.	JOB31A

where xx is the MP number
yy is the job list number
z is a letter from A to Z corresponding to the number of times that SJByy command has been given, i.e. 1 to 26 measurements.

2.1.1. *Software organisation*

The assembly of channel sets, measurement parameter lists, and job lists is exactly as described in paragraph 1.5. These data are stored in the parameter bank of the microprocessor (RAM), and must be read out separately to any data stored in the computer databank. It is possible to load new measurement data to the parameter bank via an X14 link program (LP list). This links the measurement parameters to correction and calculation parameters which will be stored in the computer databank.

The computer software programs are on the **system** flexible discs (two), and the programs are organised in modules, as below:

Disc labelled "AN"
- assembly (AS), to build up, change, or delete the information in databank and parameter bank e.g. link program, correction and calculation parameters, and other lists.
- analysis (AN), to start calibration procedures, measurement and calculation of concentrations, and related functions.
- initiation and a few reset procedures.
- hardware test (HT), see the Service Manual.

Disc labelled "UP"
- update (UP) to manipulate the contents of the files stored in the "files" disc.
- regression (RG), to calculate the instrument and sample dependent constants, using calibration values from a range of standard samples.

Some routines are present on both discs, for example, initiation, copy etc.

Note that all assembly and most measurement commands used in the microprocessor software, paragraph 1.2., can also be used in the AUTomatic mode, i.e. given from the computer terminal with asterisk (*) dialog.

The survey of commands listed in paragraph 2.2. is generally as the module listing shown above, but the grouping is functional and a particular command may not be in the headed software module, or it may appear twice in the survey. Note that a number of microprocessor commands (parameter setting, goniometer position, etc.) can only be given in the MANual mode i.e. using the microprocessor C = dialog.
In this case the computer is not used except to transmit data between the microprocessor and the computer terminal.

Initiation of the XR14 software is simple and is described in paragraph 2.1.2. After initiation any of the commands listed in paragraph 2.2. can be given. As mentioned above, the MAN command is given to revert to microprocessor (C =) only dialog.

The two station disc unit will normally be loaded with two flexible discs:
- a **system disc** (AN or UP) in station 0, containing the X14 programs.
- a **files disc** in station 1, which can contain one or more databank files (including parameter bank data), regression, recalibration and measurement results, etc.

A typical files disc readout is shown in figure 2.1A.

```
* PRD 1                          Print directory of files

LABEL = FILES                        DATE =  23  03  79  F1  PACK NBR =  100

USERID= XR-DATA                 Label and Pack number data input by IND command

1400DB  UF      2
1400PB  UF      5
STLR50  UF      7
STLB50  UF      8               Files identification, UF = users file,
CSTC03  UF      9               and first granule number of file (file may extend over
STS54A  UF     10               several granules but not necessarily in sequence).

 51 FREE GRANULES (-)           } Remaining space in disc
Indication of files used, and space remaining
**********-----------------------------------------------------------------------------
```

Figure 2.1A. Readout of files disc contents.

The following terminology is used with the X14 software, which may appear in some readouts:

Disc	— Flexible (floppy) disc (disk) mounted in the disc drive unit in station 0 or 1.
Granule	— A sub-division of the disc, there are 61 usable granules per disc.
File	— A set of records covering a **whole** number of granules, i.e. a file can be one or more granules.
Record	— A sub-division of a file. Each record contains data of one sample (C, R and B files). The length of the record is variable (in words), and depends on the number of channels measured. The number of records in a file depends on the length of a record — 1200 words are available in the first granule of a file, and 1600 words are available in the following granules.
Word	— 16 bits.

2.1.2. *Computer and disc operation*

The P851M-Computer and P830 disc drive unit are housed in a separate cabinet, and the assembly is the PW 1790/10 computer system, see figure 2.1B.

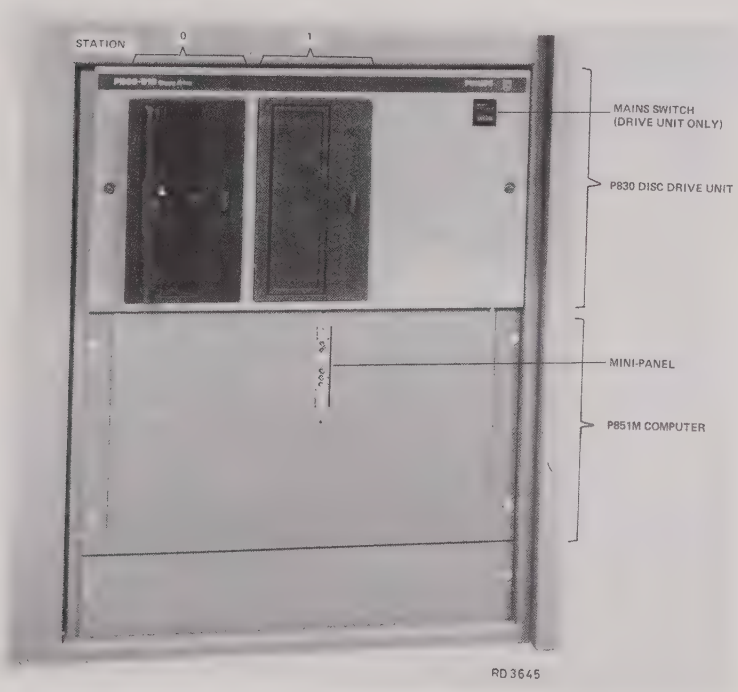


Figure 2.1B. Computer and disc drive unit.

After initiation and for normal operation, the computer cabinet door is closed.

Start-up and initiation

Before using the computer it is preferable that the disc drive unit mains switch is on (power is not yet applied to the unit). Now operate the mains switch at the top left of the PW 1790 cabinet, to apply power to the computer and the disc drive unit when the H.T. generator mains is switched on.

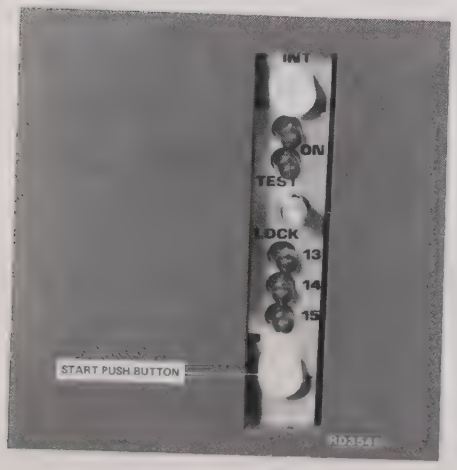


Fig. 2.1C. Computer mini-panel.

When the computer is switched on the following red lamps will be lit:
Mains switch — top panel of cabinet
Mains switch — disc drive unit
Lamp on each disc drive station (0 and 1)
Lamps on the computer mini-panel

Set the mini-panel central three-position switch upwards to TEST, see figure 2.1C. A test routine is activated and lamps 13, 14 and 15 will flash. Any error will interrupt the test routine, and the following indication will be given.

Lamp 13	14	15	Meaning
0	0	1	CPU error
0	1	0	CU error
0	1	1	Memory error
1	1	0	Bus error
1	0	0	System OK
1	1	1	LED's OK, when power switched on.

1 = lamp lit, 0 = extinguished.

Set the three-position switch to its central position. The test routine stops and the lamps will no longer flash.

Open the door of the left-hand disc drive station (0) and insert the X14 system disc (AN), with the disc label to the left and front. Close the door over the disc.

Operate the START push-button on the mini-panel (only operative with the three-position switch centralised).

The dialog DATE: and TIME: requests an input, similar to that shown in figure 2.1D, i.e. the date format is day, month and year, and the time format is hours and minutes (24 hour clock), alternatively a carriage return can be given.

The initiation program will start after the above inputs, and when it is completed the system program reference is printed "X14-xxx", and asterisk dialog is possible. xxx is the software reference number.

Now set the three-position switch to LOCK, which starts the real-time clock, and the CPU is in the "run" mode. The computer operation (measurement, printout) can be stopped by operating the INT (top) push-button of the mini-panel.

Changing a system disc

The X14 software programs are written on two system discs, although for most operation the AN disc, with the analysis and assembly modules, will be used. If it is required to change discs for regression, to update a "file" disc using the UP system disc, or to use the AN disc after using the UPdisc, the following procedure should be used:

— Give the command ENDto stop computer operation
— Remove the system disc and replace with the new disc (label to the left and front).
— On the mini-panel place the three position switch to its central position, and operate the START push-button.
— When the system is initiated input the date and time, or give carriage return.
— Place the three-position switch to LOCK, and the sytem is ready for normal operation

Insert system disc and operate START push-button

DATE :23 03 79	Input day, month, and year
TIME :16 02	Input hour and minutes (24 hour clock)
X14-AN-00.0	X14 initiation program runs, from AN disc, and serial number of software is shown.
*	Asterisk mode conversation when initiation correct.

Figure 2.1D. Initiation readout.

Initiating a new (files) disc

When a new flexible disc is to be used (as a files disc), it **must** be premarked to allow the retrieval of information. This procedure is not necessary for a new disc which is used to **copy** an existing X14 disc.

Proceed as follows:

- Ensure that the UP system disc is in station 0, if not follow the change system disc procedure above.
- Insert the new disc in station 1 (label to the left and front). Close the doors.
- Give the command IND. The dialog requests two inputs to identify the disc, LABEL = and PACK NBR =, see figure 2.1E. It is suggested that these identifications are printed on the flexible disc label.
  An asterisk will be typed when the routine is complete.
- Change the system disc — if required.

The system is now ready for normal operation.

```
DATE :23 03 1979
TIME :15 47
X14-UP-00.0
```

AN system disc replaced by update disc (UP), and initiation procedure as before.

A new disc is inserted in station 1.

```
* IND
```

Initialise the disc in station 1

```
LABEL= FILES
PACK NBR= 100
*
```

Disc identification — printed in directory (PRD) readout — see figure 2.1A.

Figure 2.1E. Files disc initiation

Switching off

Before switching off the system or PW 1790/10 it is good practice to open the doors of the two disc drive units to ensure that data on the discs are not affected in any way, also when switching on.

Selection of input and output peripherals

When the system is first used, or when the type of terminal is changed, the system parameters must be defined by typing the command ASP, see figure 2.1F. The terminal type used to input data and the output device must be defined, plus an optional second output device.

Input and output can be on the same device (output device = TT) or on separate devices (output device = RT). The latter is called **remote terminal**; for example if data is input from a VDU (terminal type = VT) a printer can be used to receive the output data (output device = RT) in which case the VDU will not display this output data.

In addition an optional **second** output device (output only) can be connected to the computer. This allows e.g. results reporting at two different locations. The commands RTM, STM and FTM apply for the transmission to this second output device.

Note that another output device can be connected to the **spectrometer (microprocessor)** interface, but this will only readout counts and time data (not concentrations, etc.), and the commands SOT and COM will apply when the system is in the MANual mode only.
The sample identification (20 characters max.) can be subdivided into separate fields up to 6. The length of each field must be input separately, but the total number of characters must not exceed 20.

Note that the ASP command input data are stored on the system disc in station 0, therefore, it is advised that the data is input on both system discs, AN **and** UP.

When the ASP command is given the following inputs can be given to define the type of peripheral and its characteristics:

Terminal type : PR = printer (PC 1409)
: VT = VDU (P817)
: GT = graphical terminal

Output devices : TT = terminal, i.e. the terminal type defined above is used for output
: LP = line printer
: RT = remote terminal (see above)

```
* PSP                          Print (existing) system parameters.
TERMINAL TYPE= VT              Video display unit used as input terminal
LINES/SCREEN=   24             24 lines per page — see paragraph 1.5.2.

CONCENTRATION AND LISTING OUTPUT DEVICES :

 1 = TT  WIDTH =  80           Output to main terminal (VDU as above)
 2 = LP  WIDTH = 130           Output to line printer — if required, see paragraph 2.4.9.

NR  IDTEXT  WIDTH              } See ASP input.
 1 IDENT      20               }

* ASP                                ASP given to change main terminal
TERMINAL TYPE= VT    :=PR            Printer keyboard used for input device
CONCENTRATION AND LISTING OUTPUT DEVICES :

 1 = TT    :=                       Printer also used to record output.
WIDTH =  80 :=
 2 = LP    :=
WIDTH = 130 :=

NR OF IDENT FIELDS = 1 :=           Maximum of 6 fields, with total of 20 characters
FIELD WIDTH 1 = 20 :=               Input number of characters in field 1
TEXT1 =IDENT     :=                 Input identification text of field 1

* PSP                          Print system parameters
TERMINAL TYPE= PR

CONCENTRATION AND LISTING OUTPUT DEVICES :

 1 = TT  WIDTH =  80
 2 = LP  WIDTH = 130

NR  IDTEXT  WIDTH
 1 IDENT      20

*
```

Figure 2.1F System parameters (peripherals) selection.

Model DJ — concentration based correction

The concentration based correction model proposed by de Jongh, in which fundamental influence coefficients (alphas) can be applied, is expressed in the formula:

$$C_i = (D_i + E_i \cdot R_i)\,(1 + \Sigma \alpha_{ij} \cdot C_j/100)$$

The corrections are based on the concentrations of the interfering elements, and the calculation uses a set of simultaneous equations.

This formula resembles the Lachance-Traill model, but includes corrections for self-absorption effects. It is extensively used and has proved successful for most applications.

The influence coefficients (alphas) are constant for a given type of sample analysis, and a given X-ray tube type and spectrometer type combination. The alphas can be calculated in the regression routine using the regression data (regression calculated alphas or experimental alphas). On the other hand Philips can provide tables with alpha values (for any combination of specified sample matrix, and spectrometer and tube type), derived from physical data (theoretical alphas). The application of theoretical alphas is extremely useful if only a small number of standard samples are available and, therefore, cannot be calculated from the regression data.

Theoretical and experimental alphas can also be used together.

Model RH — concentration based correction

The correction model proposed by Rasberry-Heinrich is expressed by the following equation:

$$C_i = (D_i + E_i \cdot R_i)\,(1 + \sum_j \alpha_{ij} \cdot C_j/100 + \sum_k \beta_{ik}\, C_k/100[1 + C_i/100]^{-1})$$

The object of the second correction term is to provide a better fit over an extra wide range of compositions. The software now includes the calculation of beta in the regression program, but theoretical values are not available.

2.1.4. **Extended calculations.**

From the concentrations results, extended calculations can be made e.g. normalisation, correction for sample dillution, and moduli calculations.
Normalisation involves the linear correction of the concentrations to bring the sum of all concentrations to a predefined value. Each concentration is there by multiplied by the normalisation factor $NF = X/\Sigma Ci$ (in which X is the predefined value). Refer to 2.4.5. **Correction for sample dillution** involves the multiplication of all concentrations with the dillution factor DF which is the final sample weight divided by the initial sample weight. Refer to 2.4.5. **Moduli calculations** involve the calculation of a linear function of the concentration (s) in the sample, which can generally be expressed as:

$$M = \frac{X_1C_1 \pm X_2C_2 \pm \text{etc}}{X_3C_3 \pm X_4C_4 \pm \text{etc}}$$

Refer to 2.3.6.

2.2. SOFTWARE COMMANDS

The X14 software commands also include a number of commands previously described in paragraph 1.2., such as assembly and analysis commands. The notes which preface paragraph 1.2 also apply, that is:

- Commands are three letter abbreviations (except stop commands).
- Commands can be followed by one or more arguments, each separated by a space (or comma).
- Commands must be terminated by a carriage return, after the last argument is given, and then the required action is initiated.
- The command listing shows the range of an argument thus: SMX i, where i must be a number from 1 to 63.
- Optional arguments are shown between brackets thus: SMX i (j) (k), means that the number for i is mandatory, but j and k are only given if required.
- In addition note that default values are shown, i.e. if an argument is not given the system will apply a given value.

A number of **PW 1400 commands** do not appear in the X14 software, and can only be given in the manual (microprocessor) mode — give command MAN. For convenience these commands are listed below:
AUT, COL, COM, CTS, DET, FLT, LWL, MSK, NRL, ORD, PCS, PTC, PTS, RMS, SCH, SCT, SLF, SLS, SOT, SSM, STS, UPL and XTL.

The software programs are on two flexible discs, and are organised in modules as listed below, but selection of a module on a disc is not necessary.

- Analysis module
- Assembly module

— AN disc

- Regression module
- Update module

— UP disc

The following survey of commands is intended to be functional, and does not necessarily relate to the order of assembly in the software modules.

Assembly

COMMAND/ARGUMENT	MEANING
ACH	Assemble a new channel. The order of the readout of channel data is the same order in which the channels sets are assembled.
ACH x(x)(i)	Assemble or change the parameters of channel xxi. The first x of a channel name must be a letter, and can be followed by an optional letter and/or a number. Up to 63 channels can be assembled. See figure 1.3A.
PCH	Print all channel data, in blocks of 5 channels, see figure 1.3B.
PCH xxi	Print the parameters of the specified channel.
PWR i k	The maximum values of the power (i) and voltage (k) of the H.T. generator are defined, where i = 0 to 3 (kilowatts) in 0.1 steps, and k = 60 or 100 (kilovolts) — for the PW 1730/10 or the PW 1732/10 generator.
ANMi	Assemble compound names, starting with combination number i. Up to 63 element/compounds can be assembled in the names list. Terminate the list assembly by a slash (/). Type DL to delete an element/compound combination.
PNM	Print element/compound names list.
AMP i	Assemble a measurement parameters list number i, where i = 1 to 63. See figure 1.3C.
PMP i	Print the measurement parameter list number i.
DMP i	Delete the measurement parameter list number i from the memory.

COMMAND/ARGUMENT	MEANING
AJB i	Assemble a job measurement program number i, where i = 1 to 63. Refer to paragraph 1.3.3.
DJB i	Delete the job measurement program number i from the memory.
■ EJB	End of a job measurement program to terminate J = input (revert to C=)

■ Means that the command can be assembled in a job list (AJB), and the job measurement commences from the SJB command or by selection from a sample changer tray identification card.

▲ Means that the command can be included in a job list, but the list cannot be selected from a sample changer card.

● Means that the command is on the AN **and** the UP system discs.

ALP i	Assemble a link program number i, where i = 1 to 63. To be linked with MP list i.
DLP i	Delete link program i.
PLP i	Print link program i.
AMB i	Assemble monitor buffer list i, where i = 1 to 63.
DMB i	Delete monitor buffer list i.
PMB i	Print monitor buffer list i.
ARC i	Assemble countrate correction set i, where i = 1 to 31.
DRC i	Delete countrate correction set i.
PRC i	Print countrate correction set i.
ACP i (xxi)	Assemble calculation parameters list i, where i = 1 to 63, from element name xxi onwards, if required. Default value for xxi in an existing CP list is the first channel.
DCP i	Delete calculation parameter list i.
PCP i	Print calculation parameter list i.
AML i	Assemble moduli list i, where i = 1 to 63.
DML i	Delete moduli list i.
PML i	Print moduli list i.
AMS i	Assemble moduli set i, where i = 1 to 63.
DMS i	Delete moduli set i.
PMS i	Print moduli set i.
ALL i	Assemble limits list (concentrations limit) i, where i = 1 to 63.
DLL i	Delete limits list i.
PLL i	Print limits list i.
● PMM	Print a memory map, of the contents of the databank.
● WDB xxxx(,i)	Write a databank having the file name xxxxDB, from the memory to the disc in station i, where i = 0 or 1. Default value of i is 0 (left-hand station).
● LDB xxxx (,i)	Load the databank with the file name xxxxDB from the disc in station i, into the memory, where i = 0 or 1 and default value is 0. Assembly data added to the databank will also be input to the LDB file, or to XR14DB if the LDB command has not been given.

COMMAND/ARGUMENT	MEANING
PPB	Print the contents of the parameter bank, to show the channel names, numbers of the MP lists and JB lists, and the remaining free space (in words) in the memory.
PPB a	Print the specified part of the parameter bank, where a = C to show list of channels a = M for MP list numbers a = J for job list numbers a = F for free space only.
DPB	Dump the parameter bank data onto disc, to preserve a record if the parameter bank is to be cleared. The RPB command is used to read the data back into the memory.
RPB	Read the data from disc into the parmeter bank.
CPB	Clear all data from the parameter bank.
• ASP	Assemble the system parameters to define input and output devices, and line widths. Default values are printer (main terminal — input and output).
• PSP	Print the system parameters.

Analysis

COMMAND/ARGUMENT	MEANING
■ SMX i (j)(k)	Start measuring unknown samples, using measuring parameter list (MP) i, and j and k if required. i (j and k) = 1 to 63. Give a space between arguments. See also paragraph 1.4.
SMA i (j)(k)	Start measurement and calculate apparent concentrations, using MP lists i, (j) and (k), otherwise as SMX.
■ SMM i (j)(k)	Start measuring monitor sample, using measuring program i, j, k. i, j, k = 1 to 63.
SPR i (j)(k)	Start prepare regression, using MP lists i, (j) and (k). First give the WDD command (or an error message will be printed), and the measured intensities will be written to the defined disc file.
i (j)(k)	Start measurement using the previously input measurement mode.
c.r.	Start measurement using the previously input measurement mode and MP lists.
SJB i (I)	Start measurement using the job program i. i = 1 to 63, with sample identification if required.

One of the following recalibration commands can be given:

SMR i	Start manual recalibration using MP list i.
SSR i	Start semi-automatic recalibration using MP list i.
SAR i	Start automatic recalibration using MP list i.

The following PWR and SPN commands can be given to set initial system conditions, and are only reset to another value.

SPN a	Set spinner to condition a, where a = Y (yes = on) or a = N (no = spinner off). The spinner will not run (a=Y) until the sample measurement commences.

When the PW1400 is switched on or reset the spinner is set to on. The SPINNER warning lamp is lit when the spinner is not running.

KVM i j	Set the H.T. generator output toi kV and j mA, where: i=25 to 100kV in 5 kV steps, and j = 10 to 80 mA in 5 mA steps. To reduce generator output values to minimum before switching off.

The following commands can be given before the start measurement commands above, to modify or extend the measurement program.

PIN	Print gross intensity measurement results in addition to the concentrations output. Reset by NPI.
NPI	No printing of gross intensities (concentrations only).
CMD	Continuous mode measurement. The cap is open during the measurement of a previously loaded sample, and this allows the continuous loading and measurement of samples. Turret positions 2 and 4 are used. Refer to paragraph 1.4.5.
/C	In continuous mode cap closes and sample passes through airlock.
BMD	Batch mode measurement. Samples are loaded into turret positions 1 to 4, before measurement, and the cap remains closed until all results are printed.
RCM i	Recycle the measurement program i times given before a start measurement command. i = 0 to 127. 0 means infinity. Refer to paragraph 1.4.6.
RCJ i	Recycle job program i times (before SJB). i = 0 to 127. Refer to paragraph 1.4.8.
MPY i	Multiply the preset time and preset count values i times, where i = in the MP lists. Refer to paragraph 1.4.6
RES	Resets all RCM, RCJ, MPY, ASC and RCS commands. The individual commands are also effectively reset when i = 1, except ASC.

The following STM and RTM commands can be given before the start measurement command to output results to a second peripheral device connected to the computer (via its interface). They do not apply to any optional output device connected to the second **microprocessor** interface, which uses the SOT and COM commands.

STM	Start transmission to a second output device connected to the computer, to print all measurment results on concentration and listing output devices 1 and 2 as specified in ASP.
RTM	Request transmission to a second output device connected to the computer. The sample measurements results are printed on concentration and listing output device 1 and the operator can decide

	whether to repeat the readout to the second device, effected by giving a carriage return.
FTM	Finish transmission, resets the STM and RTM command

The following commands can be given in addition to the above sample measurement commands.

■ CAN xxi	Calibrate the angle of channel xxi, where xxi is the name of the channel - see ACH command. Refer to paragraph 1.4.10.
PHD (xxi)	Pulse height distribution readout of the channel xxi, where xxi is the name of the channel see ACH command. Refer to paragraph 1.4.11. and 2.4.10.
SLP i	Turret sample position i to loading position, where i = 1 to 4. Cap is open.
▲ SMP i	Turret sample position i to measuring position, where i = 1 to 4. Cap is closed.
▲ LDM i	Load monitor sample in turret position i, where i = 1 to 3 (BMD), 1 and 3 (CMD).
▲ ULM i	Unload monitor sample in turret position i, where i = 1 to 3. Cap is open.
WDD (xxx)(,i)	Write measurement results to the disc in (disc drive) station i, with a file name xxx, where i = 0 or 1. Default disc station value is 1. Default file name is the one previously given.
NDD	No data to disc, to reset WDD.
ONL	On-line mode, to connect the spectrometer on-line after the error message SPECTROMETER OFF-LINE.
MAN	Manual mode, to switch to microprocessor control (C=) software control. Reset to computer control (X- 14 * mode) by command AUT.
END	End the X14 computer software operation

The following commands can be used when a sample changer is installed, refer to paragraph 3.

▲ LTU i	Load sample from the changer into turret position i, where i = 1 to 4.
▲ UTU i	Unload sample from turret position i to the changer, where i = 1 to 4.
▲ STY i	Search for tray number i = 1 to 165 (loaded on tray program card). The changer will search until position 1 of the selected tray number i is in position ready to be loaded into the spectrometer.
▲ MTY i	Move the tray to bring the sample position i ready for loading, where i = 1 to 6.
▲ FRT	Fetch the tray of reference samples, stored in the PW 1500/00 six-position changer, with reference tray option PW 1505/00. Refer to paragraph 3.1.

▲ SRT	Store the reference tray (PW1500/00 with reference tray option PW1505/00).
ASC i (j)	Automatic sample changer to be used for the measurement of samples up to, and including tray i, where i = 1 to 165. The optional argument j is an identification number from 0 to 999, which is raised by 1 for each new sample loading.
RCS i	Recycle sample changer measurements i times. i = as RCM command.
PTY i	Programmed tray i, where i = 1 to 165, can have a separate measurement program and sample identification for each sample.

Stop commands

/	Stop measurement program (or other action) immediately slash **and** carriage return given.
/S	Stop the scaler/timer operation and print the results. If a further measurement is programmed this will start after the printout of the results.
/M	Stop after the completion of the measuring program of the samples. Used to interrupt a recycling program, or to interrupt a measurement routine using the automatic sample changer. The original recycling command is not reset.
/T	Stop after the complete measurement of samples in a tray in the loading position of the automatic sample changer. The next start measurement command will commence measurement of the samples in the next tray.
BREAK or INTERRUPT	Stop immediately, interrupt any action. This action is preferred over /c.r.

COMMAND/ARGUMENT	MEANING
Regression	
SPR i (j) (k)	Start prepare regression - see Analysis commands
ACD (i)	Assemble concentration data starting with sample number i, where i = 1 to 63. Default value is 1. See also Update commands.
SRI	Start regression input of intensity and concentration values from disc file opened with OPF command. Maximum number of samples is 99, the maximum number of elements is 20 or 1200/number of samples.
SRA	Start regression analysis.
PRL (i) (j)	Print list of calculated concentrations for all samples (no arguments) or for sample (i), or for samples (i) to (j).
DSA i (j)	Delete sample i from regression calculation, or samples i to j.
ISA (i) (j)	Insert all samples (no arguments) in the calculation, or sample (i), or samples (i) to (j).
CCD i	Correct concentration data of regression element in sample i, for **LP calculation models.**
CCD i xxi	Correct concentration data of element xxi in sample i, for **DJ and RH calculation models.**
CID i	Correct intensity data of regression element in sample i, for **DJ and RH calculation model.**
CID i xxi	Correct intensity data of regression element xxi in sample i, for **LP calculation model.**
FAL xxi (r)	Fix the alpha of element xxi to the value (r). Default value of r is the previously input or calculated value.
FBT xxi (r)	Fix the beta of element xxi to the value r. Default value of r is the previously calculated value.
CAL xxi (r)	Calculate the alpha of element xxi, with a starting value of (r). Default value of r is zero.
CBT xxi (r)	Calculate the beta of element xxi, with a starting value of (r). Default value of r is zero.
RCF (xxi)	Reset correction factor of element (xxi), to reset the alpha or beta values input from CAL, FAL, CBT and FBT commands. If the element name is not given all correction factors are reset to zero.
CEB	Change equivalent background.
SRR i	Save the regression results in the CP list i. If i is given for a new CP list an identification name can be input.
NRE	Next regression element, the next element name for regression analysis can be input.
SRP (i) (tt)	Start regression analysis and print intermediate results, where (i) is the number of iterations and (tt) is the tolerance.
PLT	Plot the results of a regression analysis

COMMAND/ARGUMENT	MEANING
Update	
• OPF xxxyyy,(i)	Open file with identification xxx and extension yyy on the disc loaded in station i, where i = 0 or 1. Default value for i is 1 (right-hand station).
ADF (xxxyyy),(i)	Add a file with identification (xxx) and extension (yyy) on the disc loaded in station i, where i = 0 or 1. If the first argument is not given the file chosen, is that given by the OPF command. The default value for i is the disc chosen by the OPF command.
CLF	Close the file opened by the OPF command.
DLF xxxxxx,i	Delete the file with identification xxxxxx from the disc in station i, where i = 0 or 1.
ACD (i)	Assemble concentration data, starting from sample (i) onwards. Default value for i is 1.
ADS x	Add a sample x concentrations/intensities to the file opened by the OPF command. Sample identification x can be up to 20 characters.
DLS i	Delete the sample number i details from the file opened by OPF.
ADC xxi	Add a channel with element name xxi to all samples of the file opened by the OPF command. Concentration/intensity values must be input.
DLC xxi	Delete the channel data for element name xxi, for all samples, from the file opened by OPF.
• PSI (i) (j)	Print the sample identifications, for all samples (no arguments), or for samples (i) to (j), or for sample (i).
• PID (i) (j)	Print the intensity data for all samples (no arguments), or for samples (i) to (j), or for sample (i).
• PCD (i) (j)	Print the concentration data for all samples, for samples (i) to (j), or for sample (i).
• PCI (i) (j)	Print concentration and intensity values for all samples, for samples (i) to (j), or for sample (i).
• PJF	Print the job file from the file previously opened by OPF.
CHI i xxi	Change the intensity data for sample number i, of the element xxi.
CHC i xxi	Change the concentration data for sample number i, of the element xxi.
IND	Initialise the disc loaded in station 1. Premarks are written to the disc.
• PRD (i)	Print the directory headings for the disc loaded in station i, where i = 0 or 1 and the default value is 0.
CPD	Copy the data from the disc loaded in station 0 to the disc in station 1.
CPF xxxxxx, i	Copy the file xxxxxx from the disc in station i, where i = 0 or 1. The system will request a new file name and disc drive station.
• CST (i) (j)	Calculate the statistics for all samples in the file (no arguments), for samples (i) to (j), or for sample (i) to the maximum number in the file.
PLS (i) (j)	Plot a spectrum of the step scan in an opened job file, with an integer or channel argument, see paragraph 2.4.7.

2.2.1. Error messages

Error messages can be generated by the microprocessor software programs, or by the computer software. The microprocessor messages can be recognised as they are prefixed by two asterisks (**), refer to the listing in paragraph 1.2.1. (pages 1-11, 1-12).

The computer messages are prefixed by three asterisks (***), and are listed below. This listing shows a letter prefix which is **not printed** but is included to indicate the severity of the error, thus:

f — means that the error is fatal, and further action is not possible. Repeat command or input after corrective action, or type correct information.
r — means recoverable error, the command is not interrupted but the correct input must be given.
w — means a warning, the command input is not interrupted but check that the data or conditions are corrected later (e.g. before analysis).

f:*** GIVE FIRST WDD COMMAND	SPR command given, but WDD must be input first.
r:*** INVALID	Incorrect answer in list assembly.
f:*** INVALID ARGUMENT	Command argument is not correct repeat command with proper arguments.
f:*** INVALID COMMAND	Command not correct, repeat with proper input.
r:*** INVALID, CORRECT VALUE :=	Argument or input value not correct.
f:*** UNKNOWN LIST	List to be changed/deleted or printed is not in the memory.
f:*** UNKNOWN FILE	File does not exist in the selected disc.
f:*** UNKNOWN CHANNEL	Channel data does not exist in the selected file or list.
f:*** NO SPACE IN DATABANK	Databank full, no space for new lists.
f:*** TOO MANY ELEMENTS IN CP-LIST	More than 63 elements in the CP list
f:*** .. IS NO JOB-FILE	File opened is not a job file.
f:*** .. IS JOB-FILE	File opened is a job file.
f:*** ERROR D1	Hardware error during a write action to the disc.
f:*** ERROR D2	Hardware error during a read action from the disc.

2.4.6. Job program

A job program can be assembled in the same manner as described for the basic (microprocessors) spectrometer in paragraph 1.3.3. Note that parameter setting commands, such as SCH, COL, etc., can be input during the job assembly in J = dialog, even though these commands are not allowed during normal computer assembly when in the asterisk (*) mode.

Job measurement is also similar to the description in paragraphs 1.4.7. and 1.4.8., but note that sample identification can be given when computer control is used. When the start job SJB command is given the job list to be used must be defined as an argument. If an "I" argument is also input the operation is the same as for the SMX command, and a sample identification (up to 20 characters) will be requested.

2.4.7. Data to disc

Concentrations or intensities which are output from an SMX command sample measurement, can also be written to a flexible disc if the WDD command has been given previously. This command requires that a file name (identification) should be input, and the system will add a file extension identification, e.g. STLC50.

Concentrations will be written to the disc when the CP list is used. In the link program list, if CPNR = 0 intensities will be recorded. Note that when CPNR = 0, the counting statistical error will be printed if the CST command is given for this disc file.

A typical readout for the write data to disc operation is shown in figure 2.4K.

```
* WDD STL,1                          Write data to disc in station 1, with identification STL.

* SMX 50                             Start measurement of unknown samples.
SAM.POS= 1 I
IDENT 1= STEEL #738

*
  MP 50  CP 50  STAINLESS STEELS                          28-03-1979 16.28
CONCENTRATIONS      STEEL #738

      SI          MN           S          P          NI          CR          MO
      0.74        0.37         0.022      0.016      0.20        16.26       0.01

      NB          TI
      0.00        0.00

DATA TO FILE STLC50,1               Output shows file name STL,
                                    file extension C50, and disc drive station number.
```

Fig. 2.4K. Write measurement data to disc.

Results from a job measurement can also be written to a disc from the WDD command. If the job list includes an SMX measurement, the output to disc is as described above. If the job list contains STS, CTS, SCT, SLF, SLS or SCH instructions the results are written to a file with the name identification as specified by WDD, and the file extension will be the job list number followed by a sequence number A to Z. A is given for the first time that data are written to the file by the SJB command, B for the second SJB data input, etc. After 26 SJB inputs a different file name should be input.

A print job file (results) PJF command can be given when the file has been opened with OPF.

A typical job file readout is shown in figure 2.4L. The results were obtained from a job list measurement which comprised a step scan from 40^{o} to $46^{o}2\theta$, with a step size of 0, 1^{o} and a 1 second measurement time per step.

```
* OPF JOB54A,1                                    Open file
  128 RECORDS OF LENGTH:    6,  65 EMPTY RECORDS. FILE DATE:28-03-79
MODE= 8  JOBNR= 54      0 CYCLES

* PJF                                             Print job file
JOB       JOBNR 54  CY   0  IDENT:                          28-03-79

  ANGLE     COUNTS      TIME      ANGLE     COUNTS      TIME
  40.000       457.    1.000     40.100       439.    1.000
  40.200       496.    1.000     40.300      1292.    1.000
  40.400      2564.    1.000     40.500      2312.    1.000
  40.600      1117.    1.000     40.700       657.    1.000
  40.800       513.    1.000     40.900       447.    1.000
  41.000       416.    1.000     41.100       440.    1.000
  41.200       527.    1.000     41.300       512.    1.000
  41.400       831.    1.000     41.500      1941.    1.000
  41.600      7186.    1.000     41.700     17420.    1.000
  41.800     20286.    1.000     41.900     12733.    1.000
  42.000      4844.    1.000     42.100      1492.    1.000
  42.200       675.    1.000     42.300       489.    1.000
  42.400       395.    1.000     42.500       406.    1.000
  42.600       416.    1.000     42.700       529.    1.000
  42.800       971.    1.000     42.900      2255.    1.000
  43.000      3211.    1.000     43.100      2222.    1.000
  43.200      1114.    1.000     43.300       853.    1.000
  43.400       773.    1.000     43.500       754.    1.000
  43.600      1390.    1.000     43.700      2375.    1.000
  43.800      2143.    1.000     43.900      1089.    1.000
  44.000       554.    1.000     44.100       384.    1.000
  44.200       337.    1.000     44.300       338.    1.000
  44.400       337.    1.000     44.500       398.    1.000
  44.600       514.    1.000     44.700       996.    1.000
  44.800      3233.    1.000     44.900      9532.    1.000
  45.000     14184.    1.000     45.100     10908.    1.000
  45.200      4994.    1.000     45.300      1665.    1.000
  45.400       672.    1.000     45.500       460.    1.000
  45.600       399.    1.000     45.700       446.    1.000
  45.800       627.    1.000     45.900       851.    1.000
  46.000       749.    1.000
```

Fig. 2.4L. Job file readout.

Plotting a step scan spectrum.

A step scan spectrum can be plotted as figure 2.4M , from an opened file, e.g. the job file 54A shown in figure 2.4L. The plot spectrum command PLS is given, with an optional argument i or xxi, where i is an integer to select a particular step scan from a series in the job file, or where xxi ± is an element channel where the scan was preceded by an SCH command. All scans in the file will be plotted if an argument is not given.

```
* PLS          Plot a spectrum (no argument = all scans in the file).
PLOTMODE:
1 = JOBFILE, ANGLE PRINTED ; 2 = JOBFILE, KCOUNTS PRINTED
PLOTMODE = 1  := Select either angle or counts as X-axis
LAY-OUT OF PLOT:
POINTS = 1; HISTOGRAM = 2
LAYOUT = 1  := Select either point plot or a histogram
ELEMENT
Y-SCALE-RANGES: .1/.2/.5/1/2/5/10/20/50/100/200/500/1000
Y-SCALE=      50.0:=20   Computer suggests full scale = 50 kcps, but 20 chosen for improved resolution
          ! FS =   20.000----------------------------------------------------------------------
   40.100 !*
   40.200 !*
   40.300 !   *
   40.400 !       *
   40.500 !      *
   40.600 !  *
   40.700 ! *
   40.800 !*
   40.900 !*
   41.000 !*
   41.100 !*
   41.200 !*
   41.300 !*
   41.400 ! *
   41.500 !     *
   41.600 !                *
   41.700 !
   41.800 !                                                    *
   41.900 !                                                      *                *
   42.000 !                  *                                 *
   42.100 !    *
   42.200 ! *
   42.300 !*
   42.400 !*
   42.500 !*
   42.600 !*
   42.700 !*
   42.800 !  *
   42.900 !      *
   43.000 !         *
   43.100 !      *
   43.200 !  *
   43.300 ! *
   43.400 ! *
   43.500 ! *
   43.600 !   *
   43.700 !       *
   43.800 !      *
   43.900 !  *
   44.000 !*
   44.100 !*
   44.200 !*
   44.300 !*
   44.400 !*
   44.500 !*
   44.600 !*
   44.700 !  *
   44.800 !          *
   44.900 !                          *
   45.000 !                                          *
   45.100 !                                *
   45.200 !                 *
   45.300 !    *
   45.400 ! *
   45.500 !*
   45.600 !*
   45.700 !*
   45.800 ! *
   45.900 ! *
SAME PLOT?= NO :=
NEXT PLOT?= YE :=N
```

* *Figure 2.4 M Plot of a step scan spectrum*

2.4.8. Statistics operation

Sample analysis results can be evaluated by using a calculate statistics command CST. This routine is a very useful extension of the normal analysis procedure, where it can show analysis results on a day, week, etc. basis. This command routine is in the update module, therefore the AN disc must be replaced by the UP disc as described in paragraph 2.1.2.

The measurement results must be in a concentrations file in the "file" disc placed in station 1. First open the file by giving the OPF command with the file identification and file extension, see figure 2.4N.

When the CST command is given the readout will show columns for each element, as follows:

MAXIMUM — maximum value (%C or kcps), and the sample number between brackets.

MINIMUM — minimum value (and sample number)

AVERAGE — the calculated average value

SIGMA — the standard deviation around the average value.

COV — the coefficient of variance.

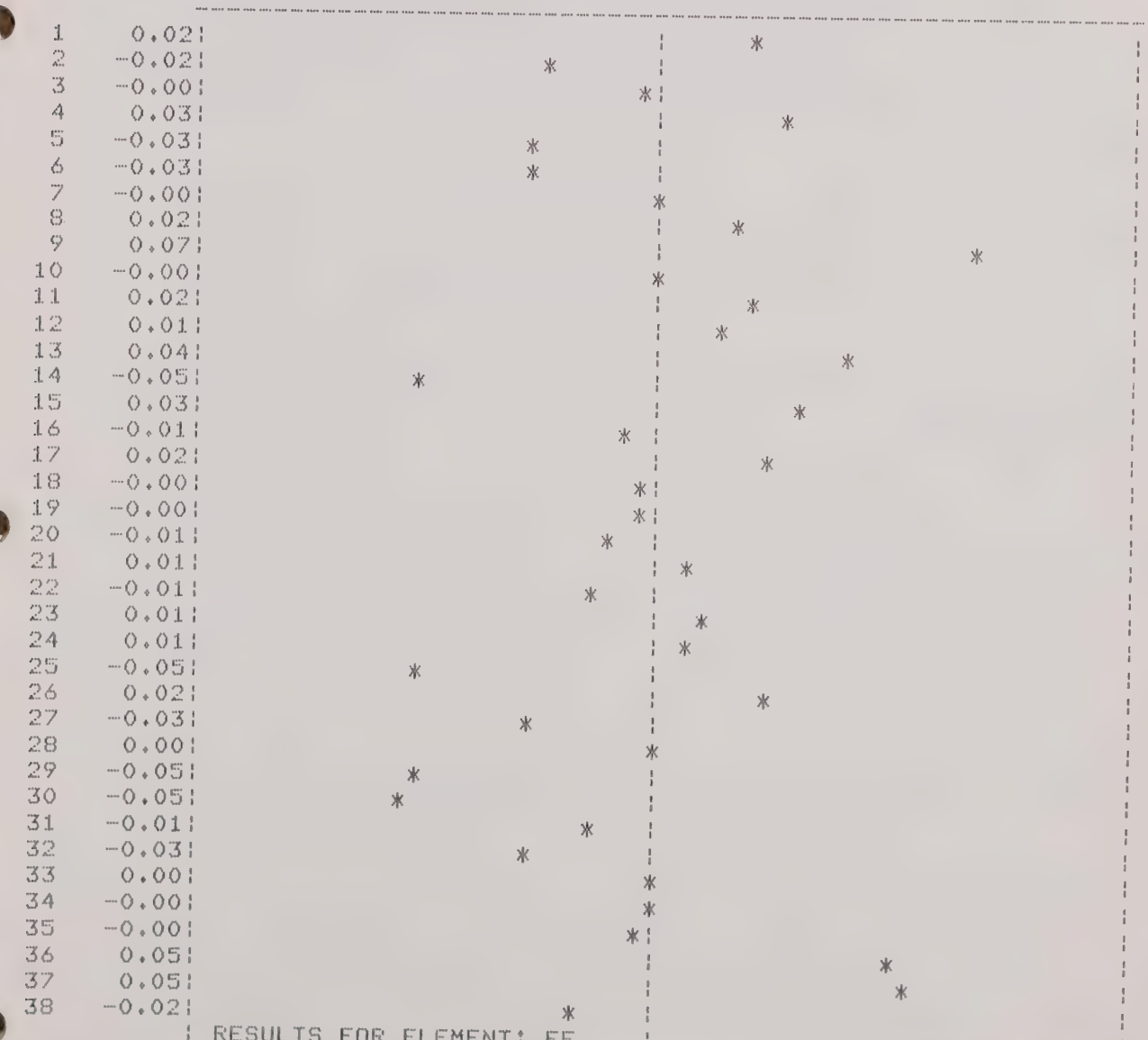
If CP = 0 in the LP list assembly (see OPF readout), there will only be intensity data in the file (in kcps), and the CST readout will additionally show the calculation of the counting statistical precision (1 sigma level) as C.ST.ERR.

If a plot of results is required type Y or YE for PLOT NO =, and the sample number and deviation from the average value (shown dotted) will be plotted, for a specified element, see figure 2.4O.

```
* OPF CSTC03,1                          Open file in disc station 1 with identification and extension.
   60 RECORDS OF LENGTH:  20,  21 EMPTY RECORDS. FILE DATE: 28-03-79
MODE= 1  MP=  3  CP=  0    38 SAMPLES Note CP = 0, results in kcps
  3 CHANNELS: NI    FE    CR
            400.0 100.0 400.0     Measurement times


* CST                                   Calculate statistics
ELM      MAXIMUM          MINIMUM          AVERAGE     SIGMA      COV     C.ST.ERR

NI      37.083 ( 14)    37.048 (  2)    37.065    0.0085    0.023%     0.026
FE     249.555 (  9)   249.252 ( 30)   249.387    0.0718    0.029%     0.020
CR      30.128 ( 13)    30.083 ( 24)    30.111    0.0104    0.035%     0.029
PLOT=NO:=
```

Fig. 2.4N. Calculate statistics.

```
* OPF CSTC03,1                                    Open file
   60 RECORDS OF LENGTH:  20,  21 EMPTY RECORDS. FILE DATE:28-03-79
MODE= 1  MP=  3  CP=  0    38 SAMPLES
  3 CHANNELS: NI     FE     CR
            400.0 100.0 400.0


* CST                                             Calculate statistics
ELM      MAXIMUM          MINIMUM          AVERAGE     SIGMA      COV      C.ST.ERR

NI      37.083 ( 14)     37.048 (  2)     37.065     0.0085    0.023%     0.026
FE     249.555 (  9)    249.252 ( 30)    249.387     0.0718    0.029%     0.020
CR      30.128 ( 13)     30.083 ( 24)     30.111     0.0104    0.035%     0.029
PLOT=NO:=Y                                       Plot results
PLOT ALL ELEMENTS=NO:=                           For defined element (s)
ELEMENT := FE                                    Results for Fe chosen
```




```
ELEMENT := /
```

Fig. 2.40 PLot element statistics results.

2.4.9. Transmission to a second output device

A second and third peripheral can be connected to the computer in addition to the main terminal, to receive output data only. Thus it is possible to transmit analysis results to a second terminal (possibly in a different location) and the operator at the main terminal can approve or inhibit the transmission to the second device.

Referring to paragraph 2.1.2., the assemble system parameters (ASP) command and input must be given before the system is used. This defines the parameters of the main terminal and the second and third (output only) devices.

Because the microprocessor software operation is independent of the computer software, it is possible to connect an output device to the microprocessor second interface (optional) and the description in paragraph 1.5. will apply, but note that only microprocessor results will be output i.e. counts and time data only.

When a second or third output device is connected **to the computer,** and is specified by the ASP command, the following commands can be used, see figures 2.4P and Q.

STM	Transmit results to a second output device. Active until reset by FTM.
RTM	Request whether transmission of analysis results to a second output device is required. After analysis and readout at the main terminal the operator can decide whether the results should be output to the second device. Active until reset by FTM.
FTM	Reset of STM or RTM command.

```
* PSP
TERMINAL TYPE= PR                          Print of system parameter

CONCENTRATION AND LISTING OUTPUT DEVICES :
1 = TT   WIDTH =  80
2 = LP   WIDTH = 130                       Line printer as second device

* RTM                                      Request transmission to second output device

* SMX 50                                   Start measurement
SAM.POS= 1 I
IDENT 1= STEEL #739


*
  MP 50  CP 50  STAINLESS STEELS                          28-03-1979 16.50
CONCENTRATIONS      STEEL #739

      SI          MN           S           P          NI          CR          MO
      0.86        1.61       0.023       0.018      20.10       25.11       0.07

      NB          TI
      0.00        0.00

START TRANSMISSION = YE :=                 Results accepted for transmission to second device.
```

Fig. 2.4P. Output at main terminal.

```
MP 50  CP 50  STAINLESS STEELS                          28-03-1979 16.50
CONCENTRATIONS      STEEL #739

      SI          MN           S           P          NI          CR          MO          NB          TI
      0.86        1.61       0.023       0.018      20.10       25.11       0.07
```

Fig. 2.4Q. Readout at second output device (output width is 130 characters per line — see PSP output, therefore the actual print out has been reduced in size).

CONCENTRATION DIFFERENCE	The difference between the chemical and calculated values.
CHEMICAL APPARENT CONCENTRATION	Equal to $C_{}/(1 + \Sigma \alpha C)$, from the correction formula $C_{} = (D + ER)(1 + \Sigma \alpha C)$
CALCULATED APPARENT CONCENTRATION	Equal to $C_A = (D + ER)$
IDENTIFICATION	Identification of the standard samples, as input by the SPR command.

When the regression results are satisfactory they can be automatically transferred to the CP list by giving **SRR** (save regression results). The regression routine then continues for the next element by giving **NRE** next regression element.

If a graphical terminal is connected the regression results can be plotted with **PLT**, which aids evaluation of the results.

2.5.1. Prepare for regression analysis

The regression analysis calculation routine requires intensity and concentration values for each element in the set of standard samples. These data are stored in a file on the files disc in disc drive 1.

When the calibration standard samples are ready for analysis, the system disc AN must be in station 0, and the files disc in disc drive 1. Give a write data to disc command WDD xxx, where xxx is a three character identification relating to the type of samples to be analysed, e.g. STL for steels as the example in figure 2.5A.

Now give the SPR (start prepare regression) command, and define the measurement/link program to be used. This number will be incorporated in the file type identification.

The dialog requests the turret positions and sample identification to be defined, and the standard samples are loaded and measured. The readout shows the intensity values which have been written to the files disc. Repeat the procedure (SPR) until all samples have been measured, then give NDD (no data to disc).

Type END, remove the AN system disc and replace with the UP (update) system disc, (files discs still in station 1), and initiate the system — mini panel switch to mid-position, operate START, input date and time or give c.r.'s, and then switch to LOCK.

The regression intensities file on the files disc must now be opened by giving the OPF xxx command, where xxx is the same identification as given with WDD above.

Now give the ACD (add concentration data) command to add the known chemical concentration values of the standard samples to the file xxx in the files disc, see figure 2.5B. The dialog will request an input of concentration values for **all** elements in all the standard samples which have been measured, so type the known value or give a carriage return (or zero).

```
* WDD STL;1
```

Write data to disc in station 1, with identification STL

```
* SPR 50
SAM.POS= 1 2 3 4 I
IDENT 1= SS-61
IDENT 2= SS-62
IDENT 3= SS-63
IDENT 4= SS-64
```

Start prepare regression

Sample loading and identification

```
*
  MP 50  CP 50                                        22-03-1979 13.08
INTENSITIES          SS-61

     MO          NB          NI          MN          CR          TI          P2
 0.03421     0.15770     0.66691     1.43867     0.92323     0.01819     0.69968

     S2          SI
 1.27439     0.36980

DATA TO FILE STLR50,1

INTENSITIES          SS-62

     MO          NB          NI          MN          CR          TI          P2
 0.05041     0.19547     1.33249     1.42797     0.76928     0.01659     0.49855

     S2          SI
 1.68475     0.36934

DATA TO FILE STLR50,1

INTENSITIES          SS-63

     MO          NB          NI          MN          CR          TI          P2
 0.03860     0.17244     1.01987     1.48324     1.06837     0.01714     0.68910

     S2          SI
 1.87100     0.38851
```

STLR50 – Note file extension

Routine continues for all samples.

Fig. 2.5A. Prepare for regression - intensities input.

```
* OPF STLR50,1
   18 RECORDS OF LENGTH: 65,    9 EMPTY RECORDS. FILE DATE:22-03-1979
MODE= 3  MP= 50  CP= 50     8 SAMPLES
  9 CHANNELS: MO    NB    NI    MN    CR .  TI    P2    S2    SI
```

Open file STLR50 on disc in station 1.

```
* ACD
```

Assemble concentrations data

```
SAMPLE  1  SS-61
MO    := .018
NB    := .000
NI    := 6.26
MN    := .78
CR    := 15.2
TI    := .000
P2    := .016
S2    := .016
SI    := .42

SAMPLE  2  SS-62
MO    := .02
NB    := .028
NI    := 12.45
MN    := .8
CR    := 12.8
TI    := .000
P2    := .015
S2    := .02
SI    := .44

SAMPLE  3  SS-63
MO    := .017
NB    := .005
NI    := 9.49
MN    := .79
CR    := 18.7
TI    :=
P2    := .016
S2    := .02
SI    := .45

SAMPLE  4  SS-64
MO    := .014
NB    :=
NI    := 20.7
MN    :=
CR
```

Continued for all samples.

Concentrations input (if available)

```
SS-66
      .43
      .006
   = 9.48
   := .81
   := 17.6
 I := .002
P2 := .02
S2 := .023
SI := .51

SAMPLE  7  SS-67
MO    := .041
NB    := 1.02
NI    := 9.52
MN    := .87
CR    := 17.8
TI    :=
P2    := .016
S2    := .018
SI    := .5

SAMPLE  8  SS-68
MO    := .033
NB    :=
NI    := 9.33
MN    := 1.59
CR    := 18.55
TI    :=
P2    := .027
S2    := .028
SI    := 1.42
```

Fig. 2.5B. Add concentrations data to file.

2.5.2. Regression analysis procedure

The intensity and concentration values for the standard samples must be input to the computer for the regression analysis routine to calculate D and E constants and matrix correction factors, see figure 2.5C.

Regression analysis is normally carried out on a regression file after the OPF command. Off-line regression analysis is possible if no file is opened using OPF before giving the command SRI.

Give the command SRI (start regression input). The dialog first requests the input (DJ, LP or RH) to define the calculation model to be used, refer to paragraph 2.1.3.

The LOAD ALL ELEMENTS request follows, and requires an answer YE (c.r. = yes), or NO if only specified elements are to be included in the routine.

After printing the list of elements that are now loaded into the computer the request REGR. ELMNT = requires an input of the first element for regression analysis. Note that the sequence of element concentrations printed after sample analysis is determined by the order of elements input to the CP list. This order is normally determined by the command SRR (save regression results) given after a regression analysis produces satisfactory results. Thus, the order of elements for the REGR. ELMNT input will determine the order of concentration result output.

```
* SRI                                    Start regression input
MODEL= DJ :=                             Select mathematical model
LOAD ALL ELEMENTS =YE:=                  Decide if all elements (on disc in station 1) to be used in regression
LOADED ELEMENTS:    MO     NB     NI     MN     CR     TI     P2     S2     S1

  8 OF THE    8 SAMPLES LOADED
REGR. ELMNT := SI                        Select first element for regression analysis

* SRA                                    Regression analysis started
ELEMENT= SI        MODEL= DJ     SIGMA=    0.01039     K=    0.01358

       D                E                Regression results for silicon
    -0.04110         1.25447

FILE:STLR50,1 (22-03-1979)
DATE:22-03-1979 13.48
```

Fig. 2.5C. Start regression input.

The command SRA (start regression analysis) starts the mathematical process of calculating the best fit for an element calibration line through the intensity/concentration points for the standard samples. The calculation takes into account any interelement correction factors which have been input.

The printout shows values for the D and E regression constants, and the goodness of fit expressed as SIGMA and K values, see figure 2.5D .

The command PRL prints a detailed list for the individual samples with respect to the calibration line. The calculated apparent concentrations can be used in the recalibration routine (paragraph 2.6), therefore, it is advisable to retain the PRL printout from the final regression (just before SRR).

If interelement corrections are applied the factors will be printed in the SRA output, see figure 2.5E. If known factors have been input these will be marked with an asterisk (from FAL and FBT). If these factors are calculated in the regression (CAL and CBT) an asterisk will not be printed.

If the calibration point for a standard sample is not acceptable, that sample can be deleted from the calculation and SRA repeated to determine whether the analysis results are improved. The PRL readout will show an asterisk against those samples which have not been included in the calculation.

```
* SRA                                          Start regression analysis
ELEMENT= SI       MODEL= DJ     SIGMA=    0.01039     K=    0.01358

      D             E
   -0.04110      1.25447

FILE:STLR50,1 (22-03-1979)
DATE:22-03-1979 13.48

* PRL                                          Print results list
NR INTENSITY -------CONCENTRATION--------  APPARENT CONCENTR. IDENTIFICATION
             CHEMICAL CALCULATED    DIFF.  CHEMICAL CALCULATED
 1    0.370   0.42000   0.42281  0.00281    0.42000   0.42281 SS-61
 2    0.369   0.44000   0.42223 -0.01777    0.44000   0.42223 SS-62
 3    0.389   0.45000   0.44628 -0.00372    0.45000   0.44628 SS-63
 4    0.391   0.45000   0.44944 -0.00056    0.45000   0.44944 SS-64
 5    0.567   0.67000   0.67015  0.00015    0.67000   0.67015 SS-65
 6    0.450   0.51000   0.52340  0.01340    0.51000   0.52340 SS-66
 7    0.439   0.50000   0.51003  0.01003    0.50000   0.51003 SS-67
 8    1.160   1.42000   1.41456 -0.00544    1.42000   1.41456 SS-68
```

Fig. 2.5D. Regression analysis for Si without interelement correction.

```
* SRA                                          Start regression analysis
ELEMENT= CR       MODEL= DJ     SIGMA=    0.11104     K=    0.02510

      D             E       ALPHA(MO )  ALPHA(NB )  ALPHA(NI )  ALPHA(MN )
   0.31563      12.48714      4.22700*    3.93200*    0.77000*    0.59000*

 ALPHA(CR )  ALPHA(TI )  ALPHA(P2 )  ALPHA(S2 )  ALPHA(SI )
   1.49500*    5.92900*    1.61300*    2.23000*    1.22600*

FILE:STLR50,1 (22-03-1979)
DATE:22-03-1979 15.06

* PRL                                          Print results list
NR INTENSITY -------CONCENTRATION--------  APPARENT CONCENTR. IDENTIFICATION
             CHEMICAL CALCULATED    DIFF.  CHEMICAL CALCULATED
 1    0.923  15.20000  15.23826  0.03826   11.81437  11.84410 SS-61
 2    0.769  12.80000  12.89799  0.09799    9.84635   9.92173 SS-62
 3    1.068  18.70000  18.63349 -0.06651   13.70531  13.65656 SS-63
 4    1.304  25.60000  25.77364  0.17364   16.48265  16.59445 SS-64
 5    1.033  18.45000  18.39801 -0.05199   13.25308  13.21573 SS-65
 6    0.943  17.60000  17.54050 -0.05950   12.12912  12.08811 SS-66
 7    0.999  17.80000  17.81247  0.01247   12.77656  12.78551 SS-67
 8    1.044  18.55000  18.40187 -0.14813   13.45755  13.35008 SS-68
```

Fig. 2.5E. Regression analysis for Cr with interelement correction.

If a HP 2648A graphics terminal is connected, plots can be produced after SRA to study the regression results, using the command PLT. (Hewlett Packard HP2648A or HP2649C).
Input to specify the X-axis and Y-axis is then requested (see fig. 2.5F), and after the input this plot appears on the screen, see fig. 2.5H and J.

```
* PLT (                                    Plot parameters
SELECT Y-AXIS:
1=CHEMC(CR  ); 2=CHEM-APPC(CR  ); 3=CALCC(CR  ); 4=CHEMC/R(CR  );
5=DIFF C(CR  ); 6=DIFF C/R(CR  )
Y-AXIS := 2                               Y-axis = chemical apparent concentrations
SELECT X-AXIS:
1=CHEMC(CR  ); 2=R(CR  ); 3=CHEMC(XX)
X-AXIS := 1                               X-axis = chemical concentrations
```

Fig. 2.5F. Plot parameters input

If X-axis 2 is selected and Y-axis 1, 2 or 3, the regression line can also be added to the plot by typing:
L carriage return. A grid can be added to the screen by typing G carriage return.
The screen is cleared with c.r. and the next plot can be made by repeating PLT.

Note that a plot can only be produced with a graphics terminal (not VDU) and GT must be specified in ASP, see fig. 2.5G.

```
* PSP                                      Print system parameters
TERMINAL TYPE= GT                         Graphical terminal specified
LINES/SCREEN =  24

CONCENTRATION AND LISTING OUTPUT DEVICES :
 1 = TT  WIDTH =  80
 2 = LP  WIDTH = 130

*
```

Fig. 2.5G. System parameters for graphical terminal.

Following the transfer of the constants to the CP list (for the first element in the regression analysis routine) the next element for analysis can be selected by giving command NRE (next regression element, see fig. 2.5R).

Note that previously input interelement correction factors are reset (in the same way as RCF), but samples deleted by DSA will remain deleted for the following analysis. If required, reinsert the stored sample intensity/ concentration values for regression analysis by giving ISA.

```
* NRE                                   Next regression element
REGR. ELMNT := CR                       Choose element for analysis

* SRA                                   Start regression analysis
ELEMENT= CR        MODEL= DJ     SIGMA=    0.72824     K=    0.17171

      D              E
   -5.36458      23.18992

FILE:STLR50,1(22-03-1979)
DATE:22-03-1979 15.03

                                        Regression analysis to follow previous element procedure
```

Fig. 2.5R. Next element for regression analysis

When all regression elements have been analysed, and the calculation parameters have been saved in the CP list on the files disc (1400 DB, 1 file), the UP system disc should be replaced by the AN disc (type END, change over the discs, operate the START switch, and then to LOCK.)
The procedure is slightly different if the databank is on the disc in station O, in which case copy the databank toDX1 after start prepare regression (SPR) input, but before the regression procedure commences with OPF and ACD. When all the regression results are satisfactory and saved, the databank on DX1 is copied to the DX0 disc.

2.6. INSTRUMENT RECALIBRATION

The DJ and RH concentration calculation models separate the constants related to the instrument (D and E), from those which are dependent on the sample (the component containing alphas and possibly betas), see paragraph 2.1.3. If major items are changed in the spectrometer system (such as the X-ray tube), or drift is experienced or suspected, it may be necessary to check and update the instrument dependent constants D and E. If monitor measurement is used, the stored monitor measurement results must be updated first, see paragraph 2.4.3., but this is not shown in the following examples.

Periodic updating of the D and E constants, for each element used in concentration calculation, can be performed by one of the following methods:

SMR — **manual input;** a set of known calibration samples are measured, and the values of **apparent** concentration are typed in. New values of D and E are calculated, and these can be saved to automatically update the associated CP list. The disc file obtained from this procedure is used during the following two methods. See paragraph 2.6.3.

SSR — **semi-automatic;** after the measurement of the known calibration samples the new D and E values are printed, and these can be saved to update the CP list. See paragraph 2.6.4.

SAR — **automatic;** after measuring the calibration samples, the computer will automatically update the stored D and E constants. See paragraph 2.6.5.

Special samples are kept specifically for instrument recalibrations, and a sufficient number should be loaded for the calculation of the D and E constants for the required elements. The number of samples can be selected by the operator dependent on the precision of recalibration required, and the time available for the recalibration routine.

The "apparent concentration" values used in the recalibration routines can be obtained by the direct measurement of the recalibration standard samples - see paragraph 2.6.2., or by using the results of measuring the calibration standard samples from the regression analysis routine — see paragraph 2.6.1.

2.6.1. Recalibration using regression analysis results

During the regression analysis routine the PRL command output will show a listing of calculated apparent concentrations, for example as figure 2.5Q. If some of these calibration standards are also used in the recalibration routine the values of **calculated apparent concentration** can be used as input for the following recalibration methods.

2.6.2. Standard samples measurement

The measurement of recalibration standard samples uses the SMA i (j) (k) command, where i (j) and (k) are MP/LP lists. With this command the measurement results readout will show a listing of the **apparent concentrations**, see figure 2.6A. Note that system disc AN must be in station 0.

```
* SMA 50
SAM.POS= 1 1
IDENT 1= RECALIBR. STAND. #1


*
  MP 50  CP 50  STAINLESS STEELS                          22-03-1979 15.21
APPARENT CONCENTR. RECALIBR. STAND. #1

     SI          MN           S           P          NI          CR          MO
     0.82        0.75        0.022       0.013       6.41        6.91        0.02

     NB          TI
    -0.02        0.04


*
```

Fig. 2.6A. Apparent concentrations readout from standard sample measurement.

2.6.3. Manual recalibration

With the SMR command a recalibration file is created in which the details of the recalibration procedure are defined, and which can be used later for semi-automatic (SSR) or automatic (SAR) recalibration. A "files" disc must be in station 1 and the AN system disc in station 0.

When the WDD command is given a file identification must also be input, and the system will add a file name extension B followed by the measurement program number, refer to figure 2.6B.
Note that the file identification can be the same as the regression analysis file, as shown in the example.
When the SMR command is given the disc file and extension identification are printed, and the dialog requests input of the sample turret loading and sample identification details. The measurement of the samples commences,to be followed by a readout of the intensities results for each sample.

After all samples have been measured the system requests an input of the apparent concentration values.

The values are obtained from the PRL list in the regression procedure - see paragraph 2.6.1., or from the measurement of standard samples using SMA - see paragraph 2.6.2.

The routine now calculates a best fit for a calibration line through the intensity/apparent concentration values. The intercept and slope values are calculated, and the printout shows the old values (from the CP list) and the newly calculated values. The operator is requested to accept (with c.r.) or refuse (with NO) the values, and if accepted the CP list values are automatically updated.

The above procedure is stored in the file specified by the WDD command, and they can be called for use in the SSR as SAR routines.

```
* WDD STL,1                          Write data to disc in station 1, with identification STL

* SMR 50                             Start manual recalibration
RECALIBRATION FILE : STLB50,1        STLB50

NR OF SAMPLES := 5                   Total of 5 recalibration standards to be used.
SAM.POS= 1 2 3 4 I
IDENT OF S  1 = SS-64                Loading and identification (first 4 samples)
IDENT OF S  2 = SS-65
IDENT OF S  3 = SS-66
IDENT OF S  4 = SS-67
*
  MF 50  CP 50  STAINLESS STEELS                                  22-03-1979 16.13
INTENSITIES        SS-64

     MO          NB          NI          MN          CR          TI          P2
   0.02929     0.15621     2.43793     1.63029     1.30457     0.01908     0.47548

     S2          SI                Intensity output in kcps.
   2.21490     0.38065

DATA TO FILE STLB50,1

INTENSITIES        SS-65           Second sample, and so on

     MO          NB          NI          MN          CR          TI          P2
   0.07158     0.16712     1.01651     1.63418     1.03230     1.34622     0.82436
```

Fig. 2.6B. Manual recalibration (page 1 of 2).

```
IDENT OF S  5 = SS-68

*        SMR example (continued)                    Loading and identification of fifth sample.
  MF 50  CP 50  STAINLESS STEELS                              22-03-1979 16.21
INTENSITIES        SS-68

      MO          NB          NI          MN          CR          TI          P2
   0.06951     0.15934     1.00619     2.66951     1.04417     0.02518     1.11366

      S2          SI
   2.49542     1.15468

DATA TO FILE STLB50,1


RECALIBRATION OF MO                    Recalibration of both or only one constant
D = YE :=
E = YE :=
USE ALL SAMPLES = YE :=                Select one or more samples
APPARENT CONCENTRATIONS:


S 1 := .0179
S 2 := .03493
S 3 := 2.46656                         Input value from SMA or regression measurement results.
S 4 := .03473
S 5 := .03751

ELM  S1 S2     D(NEW)      D(OLD)      E(NEW)      E(OLD)
MO    0  0    0.00238    -0.00061     0.43749     0.43359  SAVE=YE :=
                                                           Save to update CP
RECALIBRATION OF NB                                        list (give c.r.) or use
D = YE :=                                                  old value (give NO)
E = YE :=
USE ALL SAMPLES = YE :=
APPARENT CONCENTRATIONS:

S 1 := -.00313
S 2 := .00527
S 3 := .00523
S 4 := 1.03785
S 5 := .00158

ELM  S1 S2     D(NEW)      D(OLD)      E(NEW)      E(OLD)
NB    0  0   -0.12369    -0.12330     0.77414     0.77359  SAVE=YE :=

RECALIBRATION OF NI
D = YE :=
E = YE :=
USE ALL SAMPLES = YE :=

APPARENT CONCENTRATIONS:
S 1 := 25.40969
S 2 := 10.53249
S 3 := 10.66006
S 4 := 10.46544
S 5 := 10.44632
ELM  S1 S2     D(NEW)      D(OLD)      E(NEW)      E(OLD)
NI    0  0   -0.12984    -0.15610    10.47550    10.50491  SAVE=YE :=
```

Fig. 2.6B. Manual recalibration (page 2 of 2).

continued for all elements.

2.7. FILES AND DISC OPERATION

This paragraph covers a number of procedures which are not part of the normal sample analysis routine, such as updating disc files, copying discs, etc.
The paragraph information also supplements the notes at the commencement of paragraph 2.1, and the paragraphs 2.1.1. and 2.1.2.

2.7.1. General

The organisation of the X14 software package allows for the provision of a databank file on the AN systems disc, and this will appear in readouts as "XR14DB". This databank is intended to hold the parameters input to the computer memory, such as link programs, correction and calculation programs, etc. However, it is also possible to store databanks on a "files" disc, in which case the initially empty file XR14DB on disc AN should be copied to the files disc by giving WDB xxxx, 1. Now give the command LDB xxxx, 1, and lists which are assembled to the computer memory are immediately transferred to the opened file, i.e. the databank file in the files disc.

When all the required lists have been assembled and stored, the parameter bank which is in the microprocessor part can also be stored in the files disc, by giving the DPB command. This extension to the X14 file is identified by PB. Thus, all the relevant analysis programs can be safely stored, and for extra security the file can be copied to another disc, see paragraph 2.7.2.

For general information the commands associated with the parameter bank and databank operation are listed below:

Microprocessor commands

PPB — Print the parameter bank contents
PPB a — Print a specified part (a) of the parameter bank
DPB — Dump the parameter bank
RPB — Read in the parameter bank
CPB — Clear the parameter bank (to zero data)

X14 software

PRD (i) — Print the directory (files listing) from the disc in station i.
CPF — Copy a specified file from one disc to the other. The identification can be changed if required.
CPD — Copy the disc data from station 0 to 1.
WDB — Write databank from the computer memory to disc, with a specified identification.
LDB — Load the specified databank from disc into the computer memory.

2.7.2. Copy entire discs

It is recommended that when the PW 1400 system is first used the system discs AN and UP are copied, and the master discs can then be kept in a safe place so that further copies can be made when the first copy discs are worn. It may also be necessary to reproduce the files disc data - see paragraph 2.7.3.

Proceed as follows:

With the UP system disc in disc drive 0, give the CPD command. The computer dialog requests that the disc to be copied must be placed in disc drive 0, and the new (clean) disc be placed in disc drive 1, see fig. 2.7A. When this action is completed give a carriage return.

When the copy routine is complete the dialog prints ANSWER =. Insert any further discs to be copied (and give c.r.), otherwise, **return the UP system disc to drive unit 0,** and give a slash (/) to terminate the copy routine.

```
* CPD

PUSH THE RETURN KEY ONLY IF THE DISKETTE TO BE COPIED IS IN UNIT 0 AND
THE DISKETTE ON WHICH THE COPY IS TO BE WRITTEN IS IN UNIT 1;
PUSH THE / AND RETURN KEY WITH THE ORIGINAL SYSTEM DISKETTE IN UNIT 0 IF NO
MORE COPIES ARE REQUIRED.
ANSWER=

ANSWER=/
```

Figure 2.7A Copy disc routine

2.7.3. Copy files

To copy certain files from a files disc, proceed as follows:

- Place the UP system disc in disc drive unit 0, and the files disc in disc drive 1. If necessary, give PRD1 to print a directory of the files disc.
- Give CPF xxxxxx,1 to copy the file into the UP disc.
  Give CPF for all files to be copied.
- Remove the files disc, insert a new disc in disc drive 1, and give IND to initiate the disc.
- Give CPF xxxxxx and this file is transferred to the new disc in disc drive 1 from the UP disc. Repeat CPF for all files to be copied.
- Give DLF xxxxxx,0 to delete the file data from the UP disc for all copied files.
- Remove the new files disc and replace by the original files disc into disc drive 1, if required.

2.7.4. Update files procedure

Various commands are available to print, correct, delete and add data which is on a files disc.
Access to a file which is to be modified is obtained from the OPF command, which must state the file identification and the disc drive station 0 or 1, if required. When the required modifications have been input the file is closed by giving CLF.

The following routines can be used:

OPF — open the designated file
CLF — close the file

Concentrations — Regression and Recalibration files

ACD — to add concentrations data to a regression intensities file (from SPR command).
PCI — print sample concentrations and intensities from a regression or calibration file.
PID — print intensities only from the file.
PCD — print concentrations only from the file.
Note that a file which has been created by SMX, using a CP list = 0 in the LP list, can have a readout from PCD, although the data are not strictly concentrations.
PSI — print a list of sample identifications.

DLC — delete channel (elements) from the opened file.
ADC — add channel (elements) to the opened file.
DLS — delete sample from the file.
ADS — add sample data to the file.
CHC — change concentration data in the file.
CHI — change intensity data in the file

Job files

PJF — print of file input from WDD
PLS — plot of step scan contained in a job file

Examples

OPF and CLF, see figure 2.7B.
The OPF output will depend on type of file, i.e. the mode designation (C = concentrations, R = regression, B = recalibration, A, B, C, etc. = job).
Give the close file command (CLF) as soon as the readouts or modifications are finished.

Concentration file (SMX)

```
* OPF CSTC03,1
   60 RECORDS OF LENGTH:  20,  21 EMPTY RECORDS. FILE DATE:22-03-1979
MODE= 1  MP=  3  CP=  0    38 SAMPLES
  3 CHANNELS: NI    FE    CR
          400.0 100.0 400.0
```

Regression file (SPR)

```
* OPF STLR50,1
   18 RECORDS OF LENGTH:  65,   9 EMPTY RECORDS. FILE DATE:22-03-1979
MODE= 3  MP= 50  CP= 50     8 SAMPLES
  9 CHANNELS: MO    NB    NI    MN    CR    TI    P2    S2    SI
```

Recalibration file (SMR)

```
* OPF STLB50,1
   18 RECORDS OF LENGTH:  65,   9 EMPTY RECORDS. FILE DATE:22-03-1979
MODE= 5  MP= 50  CP= 50     8 SAMPLES
  9 CHANNELS: MO    NB    NI    MN    CR    TI    P2    S2    SI
            0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
            D  E  D  E  D  E  D  E  D  E  D  E  D  E  D  E  D  E
```

Job file (SJB)

```
* OPF JOB54A,1
  128 RECORDS OF LENGTH:   6,  65 EMPTY RECORDS. FILE DATE: 28-03-1979
MODE= 8  JOBNR= 54     0 CYCLES
```

Fig. 2.7B. Open file commands.

ACD - see figure 2.7C.

To add concentration data to a regression intensities file opened with OPF. Element concentrations must be input.

```
* OPF STLR50,1                    Open regression file
   18 RECORDS OF LENGTH:  65,   9 EMPTY RECORDS. FILE DATE:22-03-1979
MODE= 3  MP= 50  CP= 50     8 SAMPLES
  9 CHANNELS: MO    NB    NI    MN    CR    TI    P2    S2    SI

* ACD                             Add concentrations data

SAMPLE  1  SS-61
MO    := .018
NB    := .000
NI    := 6.26
MN    := .78
CR    := 15.2
TI    := .000
P2    := .016
S2    := .016
SI    := .42

SAMPLE  2  SS-62
MO    := .02
NB    := .028
NI    := 12.45
MN    := .8
CR    := 12.8
TI    := .000
P2    := .015
S2    := .02
SI    := .44

SAMPLE  3  SS-63
MO    := .017
NB    := .005
NI    := 9.49
MN    := .79
CR    := 18.7
TI    :=
P2    := .016
S2    := .02
SI    := .45

SAMPLE  4  SS-64
MO    := .014
NB    :=
NI    := 20.6
MN    := .85
CR    := 25.6
TI    := .46
P2    :=
S2
```

Concentrations data input - normally from certified calibration measurement.

and continued for all samples.

Fig. 2.7C. Concentration values added to file

```
* ANM 1
```

Assemble names, from combination 1

```
    ELM,COMPOUND
 1=     ,          := NA,NA2O
 2=     ,          := MG2,MGO
 3=     ,          := AL,AL2O3
 4=     ,          := SI,SIO2
 5=     ,          := S,SO3
 6=     ,          := K,K2O
 7=     ,          := CA2,CAO
 8=     ,          := FE,FE2O3
 9=     ,          := C3,C3S
10=     ,          := C2,C2S
11=     ,          := CC,C3A
12=     ,          := CF,C4AF
13=     ,          := LS,LSF
14=     ,          := /
```

Listing of channel/moduli names

```
* PNM
```

```
      1       2       3       4       5       6       7       8       9       10
 0   NA      MG2     AL      SI      S       K       CA2     FE      C3      C2
       NA2O    MGO     AL2O3   SIO2    SO3     K2O     CAO     FE2O3   C3S     C2S
10   CC      CF      LS
       C3A     C4AF    LSF
```

Sample measurement and results output

Note that calculation parameters list CP10 was assembled by a regression routine — not shown here. Regression analysis is shown in the stainless steel example in paragraph 2.8.2.

```
* SMX 10
SAM.POS= 1 I
IDENT 1= C 2476/27
```

Start measurement of unknown samples
Load sample
Sample identification

Results output showing moduli

```
* MP 10  CP 10  CEMENT ANALYSIS                          22-03-1979 09.55
CONCENTRATIONS     C 2476/27

      CAO       SIO2      AL2O3      FE2O3       SO3        MGO       NA2
     64.3       21.4        5.5        3.3       2.1        1.7       0.6

      K2O        C3S        C2S        C3A      C4AF        LSF
     0.39       57.4       18.1        9.0      10.0       93.6

*
```

2.8.2. Stainless steel analysis

Measurement program (MP/LP50) for stainless steel analysis, showing:

AMP	PMP		measurement program
ALP	PLP		link program
AMB			monitor buffer
ARC	PRC		countrate correction (line overlap)
LDM	SMM	ULM	monitor measurement
WDD	SPR	NDD	regression intensities

END, replace AN disc by the UP disc, and operate START push-button

OPF	ACD		regression concentrations
LDB			load databank
OPF	SRI		regression input
SRI			regression input
SRA			regression analysis
PRL			regression list printed
CCD			correct concentration input error
CAL			calculate alpha
FAL			enter known alpha value
SRR			save regr. results in CP-list
NRE			next regression element
WDB			write databank from memory

END, replace UP disc by AN disc (after satisfactory regression results), and give START

LDB			load databank to the memory
PCP			print CP list made by SRR
LDM	SMM	ULM	monitor update
SMX			measure unknowns, concentrations
PIN			print also gross intensities
WDD	SMR		manual recalibration
NPI			no printing of gross intensities
WDD	SAR		automatic recalibration
PCP			print CP-list from SAR

```
* AMP 50

MASK :  1 :=
ABS  : YE :=N
BRAT : NO :=Y
MOPS :  1 :=
MOMPY:  1 :=2

CHAN    PT    PC
          0  0E0 :=MO 10
          0  0E0 :=MO+ 2
          0  0E0 :=NB 10
          0  0E0 :=NI 20
          0  0E0 :=MN 10
          0  0E0 :=CR 20
          0  0E0 :=TI 4
          0  0E0 :=P2 10
          0  0E0 :=P2+ 4
          0  0E0 :=S2- 4
          0  0E0 :=S2 10
          0  0E0 :=SI 20
          0  0E0 :=/
```

```
* PMP 50

MP 50

MASK :  1
ABS  : NO
BRAT : YE          Buffer ratio mode
MOPS :  1
MOMPY:  2          Monitor measurement time doubled

CHAN    PT    PC
MO      10   0E0
MO+      2   0E0
NB      10   0E0
NI      20   0E0
MN      10   0E0
CR      20   0E0
TI       4   0E0
P2      10   0E0
P2+      4   0E0
S2-      4   0E0
S2      10   0E0
SI      20   0E0
```

* Channel assembly not shown

```
INTENSITIES          SS-64

      MO          NB          NI          MN          CR          TI          P2
 0.04269     0.15534     2.43370     1.67569     1.30365     0.02112     0.45612

      S2          SI
 2.03435     0.39103

DATA TO FILE STLR50,1

* SPR 50
SAM.POS= 1 2 3 4 I
IDENT 1= SS-65
IDENT 2= SS-66
IDENT 3= SS-67
IDENT 4= SS-68
```

Start prepare regression for the next four samples

```
*
  MP 50  CP 50                                        22-03-1979 13.32

INTENSITIES          SS-65

      MO          NB          NI          MN          CR          TI          P2
 0.08196     0.16621     1.01748     1.68707     1.03307     1.34631     0.82288

      S2          SI
 2.30731     0.56697

DATA TO FILE STLR50,1

INTENSITIES          SS-66

      MO          NB          NI          MN          CR          TI          P2
 5.69006     0.16615     1.02963     1.40915     0.94277     0.03663     1.21529

      S2          SI
 2.25580     0.44999

DATA TO FILE STLR50,1

INTENSITIES          SS-67

      MO          NB          NI          MN          CR          TI          P2
 0.08149     1.50100     1.01110     1.58462     0.99862     0.02846     0.61050

      S2          SI
 1.40524     0.43933

DATA TO FILE STLR50,1

INTENSITIES          SS-68

      MO          NB          NI          MN          CR          TI          P2
 0.08792     0.16143     1.00928     2.70226     1.04383     0.02440     1.09797

      S2          SI
 2.37763     1.16038

DATA TO FILE STLR50,1
```

Repeat procedure until all standard samples are measured.
No data to disc - to reset WDD.

```
* NDD
```

The regression file (STLR50), with the intensity data is now completed by manually input concentration data, obtained from certified composition figures. Replace the AN system disc in station 0, by the UP system disc- see paragraph 2.1.2. "Changing a system disc".

```
DATE :23 03 79
TIME :13 35
X14-UP-00.0

* OPF STLR50,1        Open regression file STLR50 of disc in station 1.
   18 RECORDS OF LENGTH:  65,   9 EMPTY RECORDS. FILE DATE:22-03-1979
MODE= 3  MP= 50  CP= 50     8 SAMPLES
  9 CHANNELS: MO    NB    NI    MN    CR    TI    P2    S2    SI

* ACD                  Add the concentration data to the file

SAMPLE  1  SS-61
MO    := .018
NB    := .000
NI    := 6.26
MN    := .78
CR    := 15.2
TI    := .000
P2    := .016
S2    := .016
SI    := .42

SAMPLE  2  SS-62
MO    := .02
NB    := .028
NI    := 12.45
MN    := .8
CR    := 12.8
TI    := .000
P2    := .015
S2    := .02
SI    := .44

SAMPLE  3  SS-63
MO    := .017
NB    := .005
NI    := 9.49
MN    := .79
CR    := 18.7
TI    :=
P2    := .016
S2    := .02
SI    := .45

SAMPLE  4  SS-64
MO    := .014
NB    :=
NI    := 20.6
MN    := .85
CR    := 25.6
TI    := .46
P2    := .012
S2    := .022
SI    := .45

SAMPLE  5  SS-65
MO    := .031
NB    := .006
NI    := 9.47
MN    := .94
CR    := 18.45
TI    := .002
P2    := .018
S2    := .023
SI    := .67

SAMPLE  6  SS-66
MO    := 2.43
NB    := .006
NI    := 9.48
MN    := .81
CR    := 17.6
TI    := .002
P2    := .02
S2    := .023
SI    := .51

SAMPLE  7  SS-67
MO    := .041
NB    := 1.02
NI    := 9.52
MN    := .87
CR    := 17.8
TI    :=
P2    := .016
S2    := .018
SI    := .5

SAMPLE  8  SS-68
MO    := .033
NB    :=
NI    := 9.33
MN    := 1.59
CR    := 18.55
TI    :=
P2    := .027
S2    := .028
SI    := 1.42

* CLF                  Close the file
```

Concentration values input for each element of sample

Input repeated for all samples

```
* LDB 1400,1
```

Start regression input (from files disc to the memory)

Select the calculation model - see paragraph 2.1.3.

```
* OPF STLR50,1
   18 RECORDS OF LENGTH:   65,    9 EMPTY RECORDS. FILE DATE:22-03-1979
MODE= 3   MP= 50   CP= 50      8 SAMPLES
  9 CHANNELS: MO     NB     NI     MN     CR     TI     P2     S2     SI
```

The regression file (STLR50), now contains intensity **and** concentration data. This data must be loaded into the memory (by SRI) so that regression calculations can be carried out by the computer.

```
* SRI
MODEL= DJ :=
LOAD ALL ELEMENTS =YE:=
LOADED ELEMENTS:    MO     NB     NI     MN     CR     TI     P2     S2     SI

   8 OF THE    8 SAMPLES LOADED
REGR. ELMNT := SI
```

Select first element for regression analysis

```
* SRA
ELEMENT= SI        MODEL= DJ      SIGMA=    0.01039      K=    0.01358
```

Start regression analysis (for Si).

```
       D              E
    -0.04110       1.25447
```

First calculation result

```
FILE:STLR50(22-03-79)
DATE:22-03-79 13.48

* FAL SI -.798

* FAL P2 -.845

* FAL S2 -.812

* FAL TI -.643

* FAL CR -.214

* FAL MN -.116

* FAL NI .265

* FAL NB -.393

* FAL MO -.349
```

Input of known (theoretical) alpha constants to improve the calculations of the D and E (instrument) constants, and hence the calculation of unknown sample concentrations.

The second regression analysis below shows an inprovement in the sigma and K values, and this readout also shows alpha values. Alphas which have not been calculated in the regression analysis routine, i.e. not calculated by the CAL command, are designated with an asterisk.
To further improve the results, try the deletion of any sample whose concentration/intensity input is suspect, e.g. if the PRL readout DIFFerence value is high.

```
*'SRA                                   Start regression analysis
ELEMENT= SI       MODEL= DJ     SIGMA=    0.00747     K=    0.00971

      D            E       ALPHA(MO )  ALPHA(NB )  ALPHA(NI )  ALPHA(MN )
   -0.05217      1.30101    -0.34900*   -0.39300*    0.26500*   -0.11600*

 ALPHA(CR )  ALPHA(TI )  ALPHA(P2 )  ALPHA(S2 )  ALPHA(SI )
   -0.21400*   -0.64300*   -0.84500*   -0.81200*   -0.79800*

FILE:STLR50(22-03-79)
DATE:22-03-79 13.51

*'PRL                                   Print results list
NR INTENSITY -------CONCENTRATION--------  APPARENT CONCENTR. IDENTIFICATION
           CHEMICAL CALCULATED   DIFF.   CHEMICAL CALCULATED
 1   0.370   0.42000   0.42014  0.00014   0.42880   0.42895 SS-61
 2   0.369   0.44000   0.42864 -0.01136   0.43970   0.42834 SS-62
 3   0.389   0.45000   0.44433 -0.00567   0.45907   0.45329 SS-63
 4   0.391   0.45000   0.45288  0.00288   0.45366   0.45656 SS-64
 5   0.567   0.67000   0.67086  0.00086   0.68459   0.68546 SS-65
 6   0.450   0.51000   0.51917  0.00917   0.52384   0.53326 SS-66
 7   0.439   0.50000   0.50782  0.00782   0.51140   0.51940 SS-67
 8   1.160   1.42000   1.41563 -0.00437   1.46199   1.45749 SS-68

* SRR 50                                Calculated values are acceptable, store constants in CP50 list
NEW LIST
NAME =                                  := STAINLESS STEELS  Identification of CP list
NDEC=    3 := 2   Number of decimals in concentrations readout
```

Note that the CP list identification is not requested in the following SRR dialogs.

```
* NRE                                   Next regression element
REGR. ELMNT := TI                       Regression analysis of Ti selected
```

Note that in this examples section the regression analysis is not shown for all elements.

2.8.3. Databank and parameterbank operation

In this paragraph the databank and parameterbank operation related to the examples given in 2.8.1. and 2.8.2. is shown.

Starting from initial start-up and the situation that nothing has yet been assembled in the databank and parameterbank, PMM and PPB read out as follows:

```
DATE :21 03 79
TIME :7 50
'X14-AN-00,0
```

Initiation

```
* PMM
XR14DB,0
LP   0
FREE SPACE   2982 WORDS
```

Print memory map, databank contents. Note that databank XR14DB is automatically loaded from the disc in station 0.

Empty databank (computer memory and disc).

```
* PPB
```

Print parameterbank contents.

```
FREE SPACE :   848 WORDS
```

Empty parameterbank (microprocessor).

```
*
```

Now, before assembly commands are input, the empty databank is copied onto the disc in station 1 and in this case the name "1400" is chosen.

```
* WDB 1400,1
```

Write databank to disc in station 1; identification 1400.

This (empty) databank is then loaded into the computer memory

```
* LDB 1400,1
```

Load databank from disc in station 1; identification 1400.

```
* PMM
1400DB,1
LP   0
FREE SPACE   2982 WORDS
```

Now databank 1400 in memory

Still empty

```
*
```

Now assembly input is given which is stored in the databank (computer memory and on disc) from commands like ALP, ACP, ARC, AML, AMS, ANM AMB, ALL.
Also, assembly input is given which is stored in the parameterbank (microprocessor) from commands like ACH, AMP and AJB.
After this assembly input, PMM and PPB read out as follows:

```
* PMM
1400DB,1
LP  0 10 50
MB 50
CP 10 50
ML 10
MS  1  2  3  4  5
LL 50
RC  1  2
FREE SPACE  2283 WORDS
```

Information in databank

A detailed readout can be obtained from PLP, PMB, PCP, PML, PMS, PLL, PRC, etc.

```
* PPB
F   F2  NA  MG  MG2 AL  SI  P   P2  S   S2  CL  K   CA  CA2
TI  V   CR  MN  FE  CO  NI  CU  CU2 ZN  GA  GE  AS  SE  BR
RB  SR  Y   ZR  NB  MO  RU  RH  PD  AG  CD  IN  SN  SB  TE
I   CS  BA  LA  CE  HF  TA  W   RE  OS  IR  PT  AU  HG  PB
BI  RA  U

MP 10
MP 50
FREE SPACE :  796 WORDS

*
```

Information in parameterbank

A detailed readout can be obtained from PCH and PMP.

The information in the databank is also present in the databankfile on disc (recorded automatically during assembly). A record on disc of the information in the parameterbank is made using DPB. The same disc station and filename as the loaded databank are used to record the parameterbank.

```
* DPB
FILE 1400PB,1

*
```

Dump parameterbank data to disc.

Disc station and filename same as databank, but different filetype identification (PB).

On the disc in station 1, two files exist now: a databank file and a parameterbank file which have the same name, but can be distinguished from the filetype identification which is added automatically by the system.

```
* PRD 1                          Print directory of disc in station 1.

LABEL = FILES                    DATE =  23  03  79  F1  PACK NBR =  100

USERID= XR-DATA

1400DB  UF      2                Databank
1400PB  UF      5                Parameterbank

 55 FREE GRANULES (-) :

*******-----------------------------------------------------------------

*
```

Each time the computer is switched off, the databank has to be read-in again using LDB 1400,1.
Note that the information in the parameterbank is neither affected by computer switch-off nor spectrometer switch-off (refer to 1.3.4.) nor loading of other databanks.
The parameterbank information can be read in from the file on disc into the microprocessor by RPB (after loading the appropriate databank).

```
* CPB                            Clear parameter bank

* PPB                            Empty parameterbank readout to show the effect of RPB.

FREE SPACE :  848 WORDS

* LDB 1400,1                     Load appropriate databank

* RPB                            Read the corresponding parameterbank from disc into the microprocessor.
FILE 1400PB,1                    Same disc and identification as the loaded databank


                                 Parameter bank data present in microprocessor
* PPB                            memory again.
F   F2  NA  MG  MG2 AL  SI  P   P2  S   S2  CL  K   CA  CA2
TI  V   CR  MN  FE  CO  NI  CU  CU2 ZN  GA  GE  AS  SE  BR
RB  SR  Y   ZR  NB  MO  RU  RH  PD  AG  CD  IN  SN  SB  TE
I   CS  BA  LA  CE  HF  TA  W   RE  OS  IR  PT  AU  HG  PB
BI  RA  U

MP 10
MP 50
FREE SPACE :  796 WORDS

*
```

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801110 PW 1400 XRA 156

Microprocessor software changes from version 1.5 to (the next (!)) version 2.0.

Product: **PW 1400 microprocessor version 2.0**
Medium: PROM
Prerequisities: PW 1400/00

NOTES: 1. Copies of this new release for existing customers can be ordered through:

Mr. G. Bouwhuis
S & I Logistics
N.V. Philips Gloeilampenfabrieken
Lelyweg 1
7602 EA Almelo
The Netherlands

Ordering code: 9430 - 900 - 85051
Price: free of charge (we will charge when V 2.0 is shipped and credit you when we receive the old PROM back from you).
Please specify on you order the customer name and spectrometer serial number.

2. Installations using a sample changer will require the PW 1502/00

3. Magnetic influence on X-ray intensity by the valves airlock-air-input (AAI) and airlock-vacuum-valve (AVV) is reduced completely by changed driving sequence ("powered as short as possible").

4. The new μ-proc. software version has to be introduced in all equipments. Units with serial nos DY 750, DY 752, DY 758, DY 759, DY 760, DY 763, DY 764, DY 765, DY 766, DY 767, DY 769, DY 770, DY 772 and higher than DY 772 are delivered with the new μ-proc. version 2.0 software.

General description of the modifications

On the CPU/PROM board the Philips sample changer software is replaced by an extended job-software, including "print-job(s)" and "update-job(s)" (change, insert and delete instructions in a job).
The commands STV and STH, used for variable setting of evacuation time and flushing time between closing the cap and the downward movement of the plunger are added.
Some errors are corrected and some improvements are made.
The possibility to extend the basic software by software on a second PROM-board is created (used for (optional) sample changer software).

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The PW1400 can be equipped with an extra PROM-board containing one of the following optional sample changer software versions:

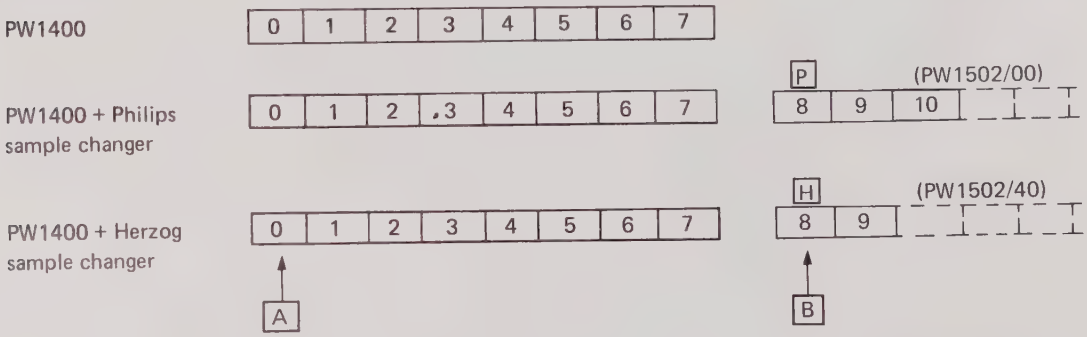
1. **PW1502/00**

Improved software version (called "VS 2.0") for the Philips sample changer PW1500/00 (incl. PW1505) and PW1500/10.
Added is software for the 12 position loader PW1506.
The software is extended by the "programmed-tray" facility.

2. **PW1502/40**

New software called ("HERZOG VS 2.0") for the Herzog sample changer:
300 position
300 position + 8 position turret
belt
belt + 8 position turret

Numbering of the proms



A = address 0000 H (till 3FFFH)
B = address 6000 H (till 67FFH resp. 6BFFH)
P = Philips sample changer software
H = Herzog sample changer software

Detailed description of the modification

1. **Basic 16 k software part**

* Sample changer software removed and thus creating free space for "print-jobs" etc.

* Job software extended:
  * print out of the contents of a joblist (PJB command)
  * change the contents of an existing joblist (using AJB command)
    * change (12 SLF 20.000: = FLT NO)
    * insert (12 SLF 20.000: = INS FLT NO)
    * delete (12 SLF 20.000: = DEL)
    * shorten list (12 SLF 20.000: = EJB)

There is a possibility to start modification directly at a given point, e.g.:

```
C = AJB  3   12     (change job 3 instruction 12)
12 SLF 20.000: = INS FLT N
12 SLF 20.000: = / (leaving remaining part unchanged)
C =
```

NOTE: the "J =" prompt is replaced by "EJB" for a new job and by the previous contents for an existing job.

* The possibility to use a second PROM-board (for sample changer software) is added.
  * board and prom's are automatically included in the PW1400 start up testprocedure if mounted in the PW1400 (termination is indicated b.m.o. "** PROMS (HERZOG) VS 2.0 CARD 2 TESTED").
  * separate prom-set for Philips and Herzog sample changer software
  * automatic rejection of sample changer commands if the second prom-board is not mounted (**COMMAND NOT AVAILABLE).

* Addition of the commands STV and STH where the evacuation time ("VACUUM") resp. flushing time ("HELIUM") between closing the cap and the downward movement of the plunger can be adjusted from 3.0 till 25.5 seconds.

* For test purposes the following testcommands are added:

  TST U — for testing μP, proms, rams, etc. without pressing the reset button or switching power off/on.

  TST B — address 1 address 2 delayfactor
  Used for testing interface boards and cabling
  (e.g. for Herzog sample changer) using a dummy plug (8 outputs connected to 8 inputs).
  All possible 8 bit codes (00 till FF) are outputted on address 1 and after delayfactor * 10 μsec. read back on address 2 and tested for equality.
  For Herzog sample changer interface board:

  ```
  C = TST  B  C080  C080  FF
  C =
  ```

* For internal use (and in combination with a special test board) a debugging package is added using interrupt level 6 (HW) or restart 6 (SW) as entry.
  The 8080 registers can be displayed/altered, software can be single stepped, etc.

  NOTE: ERROR F6 is not existing anymore!

* Some errors are corrected:
  * CTS after XTL movement in a JOB started immediately without waiting for XTL-ready.
  * After executing a measuring program containing 126 (!) channels the software continued erroneous execution of the next measuring program in memory.
  * If after the CAN-function the question "SAVE = YE :=" was not answered by Y(ES), N(O) or return but by erroneous input it was not possible to type in the correct answer afterwards.
  * RAM-test: decoder errors on RAM's 4 MSB's were not found.

* Some modifications are made:
  * "clear screen" ascii character is not stored in the input buffer anymore. Starting on a cleared screen without getting an error message is easier now.
  * "manual" start of a monitor measurement (SMM) or a job (SJB) if the PW 1400 is in ASC-mode is now possible.
    NOTE: SMX starts sample changer (!) (in ASC mode)

* ULM now only resets the monitor loaded bit su UTU can be used to unload a (formerly) monitor to the sample changer (this also applies to LTU and LDM).

* Some sample changer error-messages are changed from error-codes to text:

  ERR S.C. CODE F0 → SC NOT CONNECTED
  ERR S.C. CODE F2 → SAMPLE IN SPECTROMETER
  ERR S.C. CODE F3 → NO SAMPLE IN SPECTROMETER
  ERR S.C. CODE F4 → FRT/SRT MOVEMENT NOT POSSIBLE
  ERR S.C. CODE F5 → SAMPLE IN SPECTROMETER
  ERR S.C. CODE F6 → NO SAMPLE IN SPECTROMETER
  ERR S.C. CODE FA → NO TRAY

* The error message "ALREADY IN MEMORY" (AJB i if JOB i already exists) is deleted.

* Added are the error-messages:

ERROR F7	if angle is outside 0 - 147.005 (SCH)
ERROR F8	if number of channels in a measuring program made < (DL!)

* Magnetic influence on X-ray intensity by the valves airlock-air-input (AAI) and airlock-vacuum-valve (AVV) is reduced completely by changed driving sequence ("powered as short as possible").

2. PHILIPS SAMPLE CHANGER PART (CARD 2) PW 1502/00

* The possibility to drive the new 12 position sample loader/changer PW 1506 is added.

* The "programmed tray" (PTY) facility is added where for one tray (traynumber can be specified) a list can be assembled where for each of the 6 sample positions in the tray individually can be specified.

  1. Measurement program - or job-number - (SMX, SJB)
  2. Monitor measurement (SMM)
  3. 12 character identification (SMX)

* The following error is corrected:
  If a measurement programnumber was read from the program-card on the tray whose number was above 63, then no error message was printed but a measurement program (i-64) was started (if available).

* No automatic (vigorous) FRT/SRT movement of the PW 1505 during power-up/starting but an error message instead if the tray is **not** in one of its final positions.
  (Move by hand if not in final position).

* Own software version number (but also called VS 2.0)

3. HERZOG SAMPLE CHANGER PART (CARD 2) PW 1502/40

* New software for Herzog sample changers:

300 position sample changer
300 position sample changer + 8 position turret belt
belt + 8 position turret

The following commands can be given:

STY	"search a sample" (300 pos.) resp. "wait for a sample" (belt) (if 8 position turret connected: automatic MTY o)
STY i	equal to STY but now maximal i empty position are skipped (300 pos)
LTU j	load a sample form the sample changer to the PW 1400 turret position j
UTU j	unload a sample from PW 1400 turret position j to the sample changer
MTY k	if 8 position turret is mounted on the "loading- station" this turret can be b.m.o. this command

NOTE: The commands UTU/LTU move to/from the sample changer if the 8 position turret is in position 0 (so this position can not be used!) and to/from the 8 position turret if the turret is in position 1 till 7.

ASC	next SMX command means start automatic sample changer measurement
ASC i	equal to ASC but with automatic sample numbering system
ASC R	reset sample changer mode to "manual"
RES	equal to ASC R but **also** resetting MPY, RCM, RCJ

Measurements can be executed "manual" (using STY, MTY, LTU, UTU etc. from keyboard), "semi-automatic" (using these commands in a job) or "automatic" (SMX after ASC command), where a "batch" of samples (1 - 999 or infinite) can be measured according to a (one) measuring program specipied in the SMX command in either batch mode (BMD - fill up the PW 1400 turret with as much samples as possible) or continuous mode (CMD - use turret positions 2 and 4 and unload/load samples during measurement of the sample in the opposite position).

NOTE 1: no recycle sample changer command possible

NOTE 2: PW 1400 internal cabling and I/O interface to Herzog sample changer can be tested using a dummy plug and the TST-B command.

Example of starting automatic sample changer measurements.

C = ASC

C = SMX mp (bsz)

IDENT = XXXXXXXXXXXX

where mp = measuring program number

bsz = batch size 0 - 999 (default 1)
if 0 → infinite

XXX = 0 - 12 character identification.

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801110 PW 1400 + PW 1600/10 XRA 157

Transmission error messages in the DEC X14D and X16D software.

The meaning of transmission error messages of the X14D and X16D software is not well known. Therefore we will give a short description.
Four type of error messages may be generated:

***	**SPECTROMETER OFF**	The carrier signal (109) as received by the computer is not on.
***	**ERROR BO**	If there is a buffer overflow; the computer did receive more then 80 characters without a carriage return or an "=" character at the end.
***	**ERROR TP**	If there was no room in the computer input ringbuffer to store the incomming characters. (Through-put error). This error occurs if the transmission baud rate is high and the μP did not see a reset of the signal DSR (107) generated by a reset of the DTR (108.2) signal of the computer
***	**ERROR TR**	If there is another transmission error. This message will be given if the baud rate of the DL 11-E card in the computer and the V24 card in the spectrometer do have different baud rates or if the spectrometer interface echoes the received characters.

After the last 3 messages an extra line of information will be given e.g.

E, R, S, C = 120140 120076 130106 −290

The left part of the first word contains the contents of the error flag, which is −1 ("377) if there is a through- put error or it is equal to the left part of the DL11-E receiver data buffer register (RBUF).
The right halve contains the ASCII code of the last received character.

The second word is equal to the contents of the DL11-E RBUF at the moment that the error occured. The right halve contains the character received at the moment that the error occured. For more info see e.g. the DEC terminals and communications handbook.

The 3d word gives the contents of the receiver status register (RCSR) of the DL11-E at the moment that the error occured. The following bits should be on:

1 DTR
2 RTS
6 Receiver interrupt enable
12 Carrier signal
13 CTS

For more info see the DEC manuals.

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The 4th word indicates the number of non processed characters −290 in the input ringbuffer.

The first 3 words are given in octal code, the last word is given in binary code.

Error D9 and ERROR DA in X14/X16

Two error messages given by the X14/X16 software for the P 851 computer are not indicated in the manuals. Bothe errors may occur when one tries to copy a diskette (CPD command). In the copy proces, the written records are compared with the original records. One sees error D9 when there is a read error for the record just written and one sees error DA if the contents of the written record is not equal to the contents of the original record.
In both cases, the copy proces should be repeated with a new diskette.

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Software Survey

810130 **PW1400/00 and PW1600/10** **XRA-162**

Subject	Action required
0. Software for XRF	Already issued: PW1400/10 – XRA 141, 142, 150, 153, 156, 157, 159, 161 PW1600/10 – XRA 157, 159, 161
1. PW1490/00 Functional differences between version 2.2 and 2.1, and 2.3 and 2.2 of X14 (FRTM)	Replace software
2. PW1490/40 Functional differences between version 2.1 and 2.0 of X14 (RT11–SJ)	Replace software
3. PW1490/40 and PW1490/50 Functional differences between version 3.0 and 2.1 of X14 (RT11–SJ)	Replace software
4. PW1490/50 and PW1690/50 X14/X16 (RT11–SJ) software for PDT system	Replace software
5. PW1490/45 X14 (RT11–SJ) software for the RL01 firm disc system	
6. PW1690/00 Functional differences between version 2.1 and 2.0, and 2.2 and 2.1 of X16 (FRTM)	Replace software
7. PW1690/40 Changes with respect to version 1.0 X16 (RT11–SJ)	Replace software
8. To use a double density floppy disc with X14/X16 software (DEC-system)	
9. Selection of input and output peripherals	
10. Service facilities (HWT-command)	
11. Description of the Multiplexer PW1716/00	
12. Remarks on the computer hardware	

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SOFTWARE FOR XRF

INTRODUCTION

When analytical software packages were first introduced as separate items we chose to handle these products as project numbers, i.e. not with a PW number reference. We are now sufficiently confident to give our XRF software packages a PW number status, and the type numbers issued to date are listed and described below.

The parameters to define a software package are primarily:
- the spectrometer for which the software has been developed;
- the functions included in the software;
- the Central Processing Unit (CPU) with which the software package is to be used;
- the software monitor of that CPU, i.e. the system software from the computer manufacturer;
- the medium on which we supply the analytical software.

These parameters are specified in the PW number; the main part of the type number defines the type of spectrometer and the contents of the analytical software, and the / part defines the CPU, the monitor, and the medium.

When a software package is delivered it will automatically be to the latest version of the software.
The various software versions will not be reflected in the PW number, but you will be informed of the software releases as they become available in the normal way (XRA). Existing customers will be able to buy upgraded software packages at a reduced price.

A **Software package under PW number**

PW1490/.. Software package (X14)

	CPU	Monitor	Medium	Version	Release date	Update number	Firmware (u-proc) prerequisites version
/00	P851	FRTM	Single density disc	02.3	30-01-'81	9430 900 85111	2.0
/40	PDP11	RT11-SJ	Single density disc	03.0	15-08-'80	9430 900 85021	2.0
/45	PDP11	RT11-SJ	RL01 firm disc	03.0	19-10-'80	–	2.0
/50	PDT11	RT11-SJ	Single density disc	03.0	19-08-'80	9430 900 85061	2.0
/74 *	PDP11	RSX11-M	RK05 firm disc	03.1	–	–	–
/75 *	PDP11	RSX11-M	RL01 firm disc	03.1	–	–	–

PW1690/.. Software package (X16)

	CPU	Monitor	Medium	Version	Release date	Update number	Firmware (u-proc) prerequisites version
/00	P851	FRTM	Single density disc	02.2	15-01-'81	9430 900 85121	2.1
/40	PDP11	RT11-SJ	Single density disc	01.1	05-08-'80	9430 900 85041	2.1
/50	PDT11	RT11-SJ	Single density disc	01.1	05-08-'80	9430 900 85071	2.1
/74**	PDP11	RSX11-M	RK05 firm disc	–	–	–	–
/75**	PDP11	RSX11-M	RL01 firm disc	–	–	–	–

* Available first quarter 1981
** Available second quarter 1981

Explanatory notes

B. P851-M computer
P = the acronym for Philips
851 = the number of the series of the processors designed by Philips DATA Systems
M = for Minicomputer

C. The FRTM-monitor
FRTM = Floppy Real Time Monitor

This FRTM-monitor is specially developed by Philips Data Systems for Philips S & I. It is a stripped version of the Basic Real Time Monitor (BRTM) with a floppy disc as system device.
The MACRO-processor generates the source module FRTMSI.
Input to the MACRO-processor is the file SYSGEN, which contains the system generation parameters.

The FRTM-monitor (FRTM01) has the following configuration:

File-code	Device	Device-address	Interrupt-level
/F0	Floppy disc	/03	5
/F1	Floppy disc	/13	5
/01	Terminal (TY)	/10	6
/02	Terminal (TY)	/10	6
/05	Terminal (TY)	/10	6
/06	Terminal (LP)	/07	13
/07	Terminal (RT)	/3C	14

D. PDP = the acronym for Programmable Data Processor
PDT = the acronym for Programmable Data Terminal

11 = the number of the series of the processors designed by Digital Equipment Corporation (DEC).

E. Monitor RT-11-SJ = Real Time Single Job (SJ) operating system

A small powerful, easy-to-use disc-based system for program development or fast on-line (real time) applications.
A MACRO assembler, linker, editer, debugger and file utility programs are included.

F. Monitor RSX-11-M = Small to Moderate – sized Real – Time Multi-programming System.

An efficient multi-tasking system suitable for controlling many processes simultaneously. Utilities include a MACRO assembler, task builder (linker), editor, debugger, and file utility programs.

PW1490/00

1. FUNCTIONAL DIFERENCES BETWEEN VERSION 2.2. AND 2.1. OF X14 (FRTM)

1.1 If a SPR or start recalibration command requires a file name, and a WDD command has not been given, the system will ask for the file name instead of printing an error message.

1.2 50 or 60 Herz can be selected in the system parameters.

1.3 System options can be given in the system parameters.
Option 0 = Reset of system options.
Option 1 = See 1.6.
Option 2 = Not used.
Option 3 = Possibility to output hard copy if terminal is a VDU.

1.4 Compound names will be printed with external elements during manual input of concentrations/intensities.

1.5 Crosses will be plotted in a regression plot instead of single dots (HP-graphics).

1.6 Control of PW1716/00 added (Multiplexer).
If system option 1 is set, and the RTM or STM is given, the system will ask to which terminals the information must be sent.

1.7 If SRR or SAR is given, the identification will be fetched from the disc file if a Philips sample changer is used.

1.8 Command ATI, PTI and DTI added (TI = Tray identification). If a sample changer is connected and a file with tray identifications exists, the identifications will be fetched from this file (if the tray number is in the file and the identification given).

1.9 Following new microprocessor command implemented
- STV (set airlock evacuation time)
- STH (set airlock helium flush time)
- PTY (program tray)

1.10 Various minor errors have been corrected.

1A. FUNCTIONAL DIFFERENCE BETWEEN VERSION 2.3. AND 2.2.

1. System options 4 added to permit SMX measurement data to be saved in the disc file.
2. Various minor software amendments.

2. FUNCTIONAL DIFFERENCES BETWEEN VERSION 2.1. AND 2.0. OF X14 (RT11-SJ)

2.1 Concentrations of external elements will now properly participate in the matrix correction procedure.

2.2 With the ASP command (Assemble System Parameter), one can change the vector-address (initial value = '300) and the external page address (initial value = '175610). The two addresses will be included in the system parameter file "SYSPAR.DAT".
This file will not be present on the original disc at delivery, causing X14 (RT11-SJ) to ask for these values the first time the system is running.
A change of these addresses will only become effective if first the file "SYSPAR.DAT" has been deleted using the command "DELETE SYO: SYSPAR.DAT". (See: "selection of input and output peripherals").

2.3 The buffer to hold the parameterbank from the microprocessor, when giving the DPB or RPB command, has been decreased, thus gaining space. The total number of bytes (1482) transmitted needs 43 lines, so total 43 x 72 = 3096 characters which requires 1548 words.

2.4 In the HWT-command (Hardware Test) all arguments are allowed; although only arguments 0, 1, 2, 3, 4 and 5 have a meaning as yet. (See description "Service-facilities (HWT-command)").

2.5 In the CST-command (Calculate Statistics), having a remote terminal (RT) or line printer (LP) and also having given the answer "NO" to the question "PLOT=", the remainder of the calculations will still be printed.

2.6 In the CST-command (Calculate statistics), the counting statistical error will not be printed for elements having a zero counting time, (e.g. Moduli, external element, element by diff.)

2.7 a. If a SPR (Start Prepare Regression) file is opened and the command DLS (Delete the Sample number) is used, a question will be asked if all intensities of sample i up to the end of the file must be omitted.
b. Concentrations will be rewritten to the SPR-file, as this file could be cleared with the DLS-command.

2.8 If more than 189 alpha's are present in a CP-list, a warning will be logged (*** too many corr. in CP-list), and only 189 alpha's will be used as corrections.

2.9 The command PCS is added, allowing the user to have a print out of concentrations of samples having a specified character string in the identification. The command will allow a search through a disc file and print the relevant samples.

2.10 The message "*** RESULTS OUT OF RANGE" will be printed only by the first output device.

3. FUNCTIONAL DIFFERENCES BETWEEN VERSION 3.0 AND 2.1 OF X14 (RT11-SJ)

3.1 Control of a 300 position Herzog sample changer is incorporated in this version. (See: Sample changer ROM and Interfacing Instruction Manual PW1502/00/40/60; ordering code 9499 303 00411).

NOTE: microprocessor software V 2.0 and PW1502/40 are required.

3.2 At the beginning and the end of a concentration message (analysis) to the second output device, two extra bytes will be transmitted. Their octal values can be specified in the system parameter (ASP-command). (See: "Selection of input and output peripherals").

3.3 If SRR or SAR is given, the identification will be fetched from the disc file.

3.4 File extensions now done properly. (ERROR D8).

3.5 Recalibration with a sample changer will now show sample identification number instead of tray number and tray position.

3.6 Compound names will be printed with external elements during manual input of concentrations/intensities.

3.7 Job cycle numbers over 127 from disc are allowed.

3.8 If a command requires an opened file and finds the file closed, the system will ask for the file name instead of printing an error message.

3.9 Crosses will be plotted in a regression plot instead of single dots (HP-graphics).

4. X14D/X16D SOFTWARE FOR THE PDT SYSTEM

4.1 The DEC programmable data terminal PDT-11/150 can be connected to the PW1400/PW1600/10 spectrometer to run the RT11 X14D/X16D software.
The PDT system must have a memory of 60K and 2 floppy disc drives.
An extra interface for the connection to the spectrometer does not have to be ordered, this goes via the standard modem interface in the PDT system. This modem interface has as first external page address 176610 and a first vector address 330.
The only extra item which must be ordered is a 1 to 1 V24 interface cable e.g. the PW1340/00. This cable connects the modem exit of the PDT system to the null modem of the spectrometer.
A baudrate of 4800 must be selected on the V24 control unit in the spectrometer.
The operator terminal should be connected to the connector "CONSOLE". A 300 baud V24 printer can be connected to the connector "PRINTER". If data is to be printed on this printer the device LP should be selected in the system parameters (listing and concentrations output device).
The cluster EIA option for 3 extra terminals is not supported by our software. Device RT can also not be selected with this system. The device name for the upper floppy disc drive is DK0 or SY0 and the name of the lower drive is DK1 or SY1.
The names DX0 and DX1 cannot be used with this system.

4.2 The boot procedure is different from other PDP11 computers:

1. Switch on the main power of the PDT-system and the operators terminal.
2. Insert the system disc in the upper disc drive.
3. Bring the mode switch on the rear panel of the PDT system to the "RESET" position.
4. Type the symbol @ twice via the operators keyboard.
5. The PDT RT-11 monitor will now be loaded, the modem baudrate will be set to 4800 baud and the printer baudrate will be set to 300 baud.
6. Load and start the spectrometer program (R PW1400)/(R PW1600).

4.3 If a printer with a baudrate of 1200 baud is connected to the connector "PRINTER", the standard STARTS.COM file should be replaced by the file STARTS.PDT. This is possible with the following RT-11 command:

RENAME STARTS.PDT to STARTS.COM

One should do this only with a copy of the original system disc because the original file "STARTS.COM" will be deleted by this operation.

4.4 Software for this system should be ordered as PW1490/50 or PW1690/50. One system disc will be delivered with the system, which contains the PDT RT-11 single job monitor and the PW1400/PW1600 program for the optional HP graphic terminal.
The VT55 terminal will not be supported in our software for the PDT system.
The following modules have been copied from the PDT disc as D983B-BC (RT2/PDT V03B BIN RX01): PDMNSJ.SYS, TT.SYS, LP.SYS, SWAP.SYS and the BOOT BLOCK from PDMNSJ.SYS.
A number of special PDT files have been added: STARTS FILES used after the start of the RT-11 monitor, program LP300B called in file STARTS.COM to select baudrate 300 for the printer, and program SPD480 to select a baudrate of 4800 baud for the modem interface for the spectrometer.

5. X14D SOFTWARE FOR THE RL01 FIRM DISC SYSTEM

5.1 The PW1490/45 consists of the X14D software version 3.0, supplied on a RL01K-DC (DEC-type number) disc. The disc contains the standard RT11 V3B monitor for the RL01 disc system and the PW1400 Load modules version 3.0.
The name of the HP2648A Load module is PW1400.SAV and the name of the VT55 Load module is PW14VT.SAV. Monitor DLMNSJ.60H is the standard 60 Hz monitor, and DLMNSJ.SYS is the standard monitor used for 50 Hz.
The file VT55.COM has been deleted; to run the VT55 version of the X14D software give the command:
R PW14VT.

5.2 **Copy entire discs.**
Proceed as follows:

- Load the system (or master) disc in the upper drive (DL0), and the new disc in the lower drive (DL1).
- Type @ COPY, where @ is the DEC writer upper case 2.
- Answer Y to the request "Init are you sure?"
  The entire contents of the disc in station DL0 are written to the disc in station DL1, and any data on the latter disc will be overwritten.
- Copying time 5—10 minutes.

```
.@COPY

.INIT/BADBLOCKS SY1:

SY1:/INIT ARE YOU SURE?Y
```

PW1690/00

6. FUNCTIONAL DIFFERENCES BETWEEN V2.1 AND V2.0 OF X16 (FRTM)

6.1

1. The microprocessor commands AMT (Assemble Monitor Tray) and MMT (Measure Monitor Tray) are added.

   NOTE: The MMT-command is a microprocessor command only.

2. The SMX-command given without argument will cause the system to use the previously input MP-number.
3. Graphics on the HP-terminal will show small crosses instead of single dots (regression program).
4. Graphics plotting can be aborted by giving an interrupt.
5. Line feed is given before the heading of the CST output.

6.2 **Corrected errors.**

1. Changes in several routines are necessary because DOS release 8 is used.
2. The answer "N" for internal ratio calculation for an element is accepted.
3. The asterisk of a command input request is always printed.
4. "MAINS FREQUENCY=" answered with a slash (/) will cause the system parameters to be written to disc.
5. Output of system parameters (when the first listing device has been defined as RT or LP) will now be on RT or LP, including the microprocessor part of this output.
6. Line printer and remote terminal now have different interrupt addresses.
7. Sample changer mode with a tray card. SMX will be excuted if the 21st character of the identification is a space.
8. PCS-command given, and INT button pushed, will abort the print operation for all samples in all files.
9. PCS-command: Even if files have a different length, all sample data will be printed.
10. Change in the "end - of - databank" search to avoid a Fortran error after a PMM command.
11. The asterisk of the out of limit check will be printed in the correct place.
12. PCI-command given after a DLS-command, and no more samples in the file, will no longer print data.
13. ALP-command: Space or comma is now accepted as a separator.

6A. FUNCTIONAL DIFFERENCES BETWEEN V2.2. AND V2.1.

1. System parameter options added (ASP dialog).
   Option 0 = Reset of system options.
   Option 1 = See 1.6.
   Option 2 = Not used.
   Option 3 = Hard copy output possibility if terminal is a VDU.
   Option 4 = Possibility to save SMX data in the disc file.
2. Various minor software amendments.

PW1690/40

7. CHANGE TO VERSION 1.0:

1. Due to an error in the routine ASPPSP, error 61 occurred during start-up when the file SYSPAR.DAT was not on the systems disc.
2. With a full databank, a check was not made in PMMCOM on searching lists outside the databank.
3. In the routine PCSCM6 a different search approach is used, thus making the routine much faster.
4. A slash given during plotting will abort the plot.
5. Output of compound names with concentration/intensity input was incorrect.

8. TO CREATE A DOUBLE DENSITY FLOPPY DISC WITH X14/X16 SOFTWARE, PERFORM THE FOLLOWING STEPS:

1. Place the standard DEC floppy with DYMNSJ.SYS in DY0.
2. Place new floppy in DY1.
3. Boot DY0.
4. When booting is ready type RUN FORMAT after the dot.
5. Type DY1 after the asterisk and ^C (CONTROL-C) behind the second asterisk.
6. Type INIT/NOQUERY/BADBLOCKS DY1 after the dot.
7. Type R PIP after the dot.
8. Remove floppy from DY0 after the asterisk.
9. Place PW1400/PW1600 floppy in DY0.
10. Type DY1:*.*=DY0:*.* after the asterisk, (ignore warning that .SYS-files will not be copied).
11. Remove floppy disc from DY0 when the asterisk appears again.
12. Place standard DEC floppy with EDIT.SAV in DY0.
13. Type DY1:EDIT.SAV=DY0:EDIT.SAV after the asterisk.
14. Remove floppy disc from DY0 when the asterisk appears again.
15. Place standard DEC floppy with DYMNSJ.SYS in DY0 again.
16. Type ^C (CONTROL-C) after the asterisk, and give the following when a dot is printed:
    DEL/NOQUERY DY1:RESORC.SAV
    COPY/SYS (DYMNSJ, SWAP, TT, LP) .SYS DY1:
    COPY/BOOT DY1:DYMNSJ.SYS DY1:
17. Remove floppy from DY0: and insert floppy from DY1: in DY0.
18. Boot DY0: (ignore warning RT-handler)
19. After the booting is ready, type EDIT STARTS.COM after the dot.
    Type RB[ESC]GUSR[ESC]GNO[ESC] = D[ESC]EX[ESC][ESC] after the asterisk ([ESC] means escape-key).
20. Type DEL/NOQUERY *.BAK,
        SQUEEZE/NOQUERY DY0:
    after the dot is printed.

9. SELECTION OF INPUT AND OUTPUT PERIPHERALS

When the system is first used, or when the type of terminal is changed, the system parameters must be defined by typing the command ASP.
The terminal type used to input data and the output device must be defined.

Input terminal type : PR = printer (PC1409)
: VT = VDU (P817)
: GT = graphical terminal

Output devices
: TT = output terminal is the same as the input terminal
: LP = output terminal is a separate printer, e.g. a Line Printer
: T1, T2, T3 = the output terminal is a separate printer, which is connected to a computer interface, which is different to LP or RT
RT = is a separate output terminal (printer), which is connected to a computer interface, which is different to LP, T1, T2 or T3

If only one terminal is used for both input and output TT must be declared.

9.1 Terminal to computer connections

Terminal code:	computer systems		
	P851/interfaces	PDP11/.. interfaces	PDT11/150 (connectors)
"spectrometer"	SALCUZ in slot 7	DL11 – E	"modem"
TT (= PR, VT or GT)	SCUZ in slot 6	DL11 – WB	"console"
LP	SCUZ in slot 8	DL11 – WB	"PRINTER"
T1	–	–	"Terminal 1"
T2	–	–	"Terminal 2"
T3	–	–	not used
RT	SCUZ in slot 9	DL11 – WB/WA	–

Take care that the jumper settings and connections (baud rate, etc.) have been correctly made.

Input and output can be on the same device (output device = TT) or on separate devices (output devices = RT) The latter is called **remote terminal**; for example if data is input from a VDU (terminal type = VT) a printer can be used to receive the output data (output device = RT) in which case the VDU will not display this output data.

In addition an optional **second** output device (output only) can be connected to the computer. This allows e.g. results reporting at two different locations. The commands RTM, STM and FTM apply for the transmission to this second output device.

RTM = Request TransMission to second terminal
STM = Start TransMission to second terminal
FTM = Finish TransMission to second terminal

If a terminal is selected, but is not addressable (such as T3 or RT with the PDT11/150), the computer returns to the DEC dot mode (•mode).

Modes of the software dialog

There are three modes of conversation:

– "Dot" • using the DEC monitor software
– "Asterisk" * using the X14/X16 software
– "C=" C= using the PW1400/1600 microprocessor software

9.2 **Start up and initiation** (DEC - PDP11/.. system)

1. Switch on the main power of the PDP11-system and the operators terminal.
2. The computer will be operational if the PDP11 control panel knob is set to DC ON. (The RUN and DC ON lamps should be lit).
3. Note that during switch on and switch off the loading flaps of the two disc drive should be open if they are loaded with a floppy disc. This will prevent any switching transients from affecting the data on the discs.
4. On the PDP11 control panel momentarily operate the BOOT key to INIT. The PDP11 internal program will run and type four groups of numbers.
5. Ensure that the system disc with the X14/X16 program is loaded into the left-hand disc drive station and the drive unit flap is closed. This disc is inserted with the label on top and to the front.
6. Type DX, and this will cause the initial program on the system disc to be read into the computer. The computer will then output the system parameters, and the time and date which are already in the memory.

```
032304 030602 001072 000030          Typical output from PDP11 internal program
@DX                                  Read in initial program from the system disc
RT-11SJ (S)V03B-00C

.SET USR NOSWAP

.TIME 09:00:00

.DATE 14-AUG-80

.INSTALL RT:

.ASS RT: 4

.SET RT CR

.SET RT LC

.SET RT NOFORM0

.SET LP NOFORM0
                                     ← Input new date and time, if required
.R PW1400       OR R.PW1600

X14D-003.0      OR X16D-001.1

*                                    Ready for asterisk dialog
```

9.3 **Start up and initiation** (DEC - PDT11/150 system)

1. Switch on the main power of the PDT11/150 system and the operators terminal.
2. Insert the system disc in the upper disc drive.
3. Bring the mode switch on the rear panel of the PDT system to the position "RESET".
4. Type the symbol @ twice via the operators keyboard.
5. The PDT RT-11 monitor will now be loaded, the modem baudrate will be set to 4800 baud and the printer baudrate will be set to 300 baud.
6. Load and start the spectrometer program (R PW1400) or (R PW1600).

```
@@                          READ IN INITIALPROGRAM FROM THE SYSTEM DISC
RT-11SJ (S)V03B-00D

.SET USR NOSWAP

.TIME 09:00:00

.DATE 12-SEP-80

.SET LP CR

.SET LP LC

.ASS PD DX

.ASS PD DX0

.ASS PD1 DX1

.R LP300B

.R SPD480

.TYPE STARTS.LS1
?PIP-F-Input error DK:STARTS.LS1

.
 R PW1400      OR  R.PW1600

X14D-003.0     OR  X16D-001.1

*                                READY FOR ASTERISK DIALOG
```

9.4 START UP and initiation (Philips P851 system)

Before using the computer it is preferable that the disc drive unit mains switch is on (power is not yet applied to the unit). Now operate the mains switch at the top left of the PW1790 cabinet, to apply power to the computer and the disc drive unit when the H.T. generator mains is switched on. Ensure that the disc drive doors are open.

Initiation

1. If a PW1790/11, with a full panel, is installed proceed as follows:
   Insert the X14/X16 system disc (AN) in station 0, and close the door.
   Set the TEST/LOCK switch to its mid-position (pull the switch spring-loaded lock to adjust its position).
   Set the data switches to /4083 (switches 1, 8, 14 and 15 up — the remainder down). If the AN disc is loaded in station 1 the switches should be set to /4093.
   Press the INST push-button, (or LR).
   Press the MC push-button.
   Press the IPL push-button. This loads the bootstrap and IPL program. The computer will start loading the program, but requests DATE and TIME inputs. The program runs, and asterisk conversation is possible. Set the TEST/LOCK switch to LOCK.
2. If a PW1790/10, with mini-panel, is installed proceed as follows:
   Set the mini-panel central three-position switch upwards to TEST. A test routine is activated and lamps 13, 14 and 15 will flash. Any error will interrupt the test routine, and the following indication will be given.

Lamp 13	14	15	Meaning
0	0	1	CPU error
0	1	0	CU error
0	1	1	Memory error
1	1	0	Bus error
1	0	0	System OK
1	1	1	LED's OK, when power switched on

1 = lamp lit, 0 = extinguished.

Set the three-position switch to its central position. The test routine stops and the lamps will no longer flash.

Open the door of the left-hand disc drive station (0) and insert the X14/X16 system disc (AN), with the disc label to the left and front. Close the door over the disc.

Operate the START push-button on the mini-panel (only operative with the three-position switch centralised).

The dialog DATE: and TIME: requests an input, i.e. the date format is day, month and year, and the time format is hours and minutes (24 hour clock), alternatively a carriage return can be given.

The initiation program will start after the above inputs, and when it is completed the system program reference is printed "XxxANxxx", and asterisk dialog is possible. xxx is the software reference number.

Now set the three-position switch to LOCK, which starts the real-time clock, and the CPU is in the "run" mode. The computer operation (measurement, printout) can be stopped by operating the INT (top) push-button of the mini-panel, by operating the "break" or "interrupt" key on the input terminal, by typing a slash c.r. (/) or by pressing the RESET push-button on the BUS INTERFACE circuit board.

If the power fails, or the computer is switched off and on, the initiation procedure must be repeated to resume asterisk dialog. It is good practice to open the disc drive doors before applying mains power.

```
DATE :18 12 80      input date, cr
TIME :15 45         input time, cr
X14-AN-02.2

*                   READY FOR ASTERISK DIALOG
```

9.5 Assemble system parameters

1. Transmission codes

A "start of transmission" code and "end of transmission" code can be required when measurement data is sent to a remote computer or terminal, after a STM or RTM command has been given. These codes are octal representations of two characters. If the dialog input is 0 (zero) a special code will not be transmitted.

The first character of the transmitted code must be given in the eight least significant bits of the code word (right byte), and the second character is in the eight most significant bits (left byte).

Example

Assume the start of transmission code is only a form feed control character. The ASC II code for this character is "014" (refer to the PDP11 programming card).
Assume the end of transmission code is an EOT control character "004", followed by a carriage return control character "015", Therefore, the end of transmission code has 015 in the left byte and 004 in the right byte, that is:
00 001 101 00 000 100 = 0 000 110 100 000 100 = 6404
(0) (1) (5) (0) (0) (4)

Therefore, the dialog input in the ASP command would be
START TRANSM CODE = 14
END TRANSM CODE = 6404

2. Vector and Address

PDP11/.. systems

Interface for	Interface Type No.	Page address	Vector (int) level
"spectrometer"	DL11-E	175610	300
Operators Terminal	DL11-WB	177560	060
Remote Terminal			
(Printer) – V24	DL11-WB		
– current loop	DL11-WA	175620	310
PDT11/150 system			
"spectrometer"	DL11-E	176610	330

If the settings have to be changed, because the default values are not possible in the configuration or because they are already used by other interfaces in the system, proceed as follows:

Switch the mains off and change the jumpers of the DL(V) 11-E card.
Start the RT11 monitor and delete file SYSPAR.DAT.
Start the spectrometer program, which will then request the system parameters.
Give the correct data for the DL(V) 11-E address and vector.

3. * ASP DEC systems

```
TERMINAL TYPE= GT    :=
LINES/SCREEN =  24  :=
CONCENTRATION AND LISTING OUTPUT DEVICES :
 1 = TT     :=
WIDTH =  72  :=
 2 = TT     :=
WIDTH =  72  :=
START TRANSM.CODE=        0  :=
END   TRANSM.CODE=        0  :=
DL(V)11-E  VECTOR =     300  :=
DL(V)11-E ADDRESS = 175610  :=

NR OF IDENT FIELDS = 1  :=
FIELD WIDTH 1 = 20  :=
TEXT1 =IDENT      :=

*
END

.DEL SYSPAR.DAT
 Files deleted:
DK:SYSPAR.DAT ? Y

.R PW1400   OR   R. PW1600

X14D-003.0  OR  X16D-001.1

*** NO SYSTEM PARAMETERS ON SY0:
TERMINAL TYPE= PR    := GT
LINES/SCREEN =  24  :=
CONCENTRATION AND LISTING OUTPUT DEVICES :
 1 = TT     :=
WIDTH =  72  :=
 2 = TT     :=
WIDTH =  72  :=
START TRANSM.CODE=        0  :=
END   TRANSM.CODE=        0  :=
DL(V)11-E  VECTOR =     300  :=
DL(V)11-E ADDRESS = 175610  :=

NR OF IDENT FIELDS = 1  :=
FIELD WIDTH 1 = 20  :=
TEXT1 =IDENT      :=

*
```

Graphics terminal

output to graphics terminal

See transmission codes 9.5.1.

Set for PDP11/ ..

Maximum of 6 fields, with total of 20 characters
Input number of characters in field 1
Input identification text of field 1

To revert to the "dot" mode (RT–11) give the END command. This may be necessary if the time and data are to be changed.

Graphics terminal

See transmission codes 9.5.1.

Set for PDP11/ ..

Maximum of 6 fields, with total of 20 characters
Input number of characters in field 1
Input identification text of field 1

4. * ASP Philips P851 system

```
TERMINAL TYPE= PR    :=
SYSTEM OPTIONS=  0 :=
MAINS FREQUENCY = 50 :=
CONCENTRATION AND LISTING OUTPUT DEVICES :

 1 = TT    :=
WIDTH =  72 :=
 2 = TT    :=
WIDTH =  72 :=

NR OF IDENT FIELDS= 1 :=
FIELD WIDTH 1 = 20 :=
TEXT1 =IDENT     :=
*
```

Printer Keyboard used for input device

0 = normal
1 = reserved for use with multiplexer (e.g. PW1716)
If option 1 is set and RTM command is given, system ask for the terminals (selected via the multiplexer) on which the data has to be printed.

Maximum of 6 fields, with total of 20 characters
Input number of characters in field 1
Input identification text of field 1

10. SERVICE FACILITIES (HWT-COMMAND)

For error-tracking the command HWT has been incorporated in the software, giving the following possibilities:

1. **Command HWT 0.** This is the default-value when starting up the X14D/X16D software. It resets the special features of the HWT-command as indicated below.
2. **Command HWT 1.** When this command has been given, the output of the spectrometer to the computer can be monitored on the terminal. It will be reset with HWT 0.
3. **Command HWT 2.** This command sets the mode to on-line (coupling of spectrometer and computer).
4. **Command HWT 3.** This command set the mode to off-line (spectrometer not connected to the computer). Input of intensities can be done from the terminal, if a measurement must be simulated without the spectrometer.
5. **Command HWT 4.** This command is used to read data from a memory-location or to write data to it. After the command the message R/W = appears, after which the following can be typed:
   a. R (arg1) (arg2)
      The R denotes "read from memory"; the arguments are not obligatory. If an argument has not been given the location whose address has been typed-in previously will be read. If the command is the first one after the HWT 4-command, the location 0 will be read.
      If only arg1 has been given, the location with that address will be read.
      If both arguments have been given, the locations from arg1 up to and including arg2 will be read.
   b. W arg1 arg2.
      The W denotes "write into memory"; the arguments are obligatory.
      The first argument arg1 denotes the address of the location to write-in; arg2 is the data to be stored in arg1 address.

Odd addresses are not allowed in HWT 4.

NOTE: HWT 4
Be very careful in using this command as when writing into the memory to wrong addresses the X14D or X16D program can be destroyed.

6. **Command HWT 5.** This command is used to change the tolerance and maximum number of iterations in the concentration calculation. It can also be used to provide the concentration values of all calculated elements after each iteration cycle (useful if ERROR EE has been printed).

11. DESCRIPTION OF THE MULTIPLEXER PW1716/00

With the multiplexer connected to the SCUZ for the remote terminal, it is possible to distribute the output to a maximum of 8 (1 multiplexer connected) or to 16 printers (2 multiplexers connected).

In the system parameters if the system-option 1 has been selected and the RTM-command is given, the dialog will request to which terminals (0 – 16) the data has to be printed. (0 means no transmission).
It is also possible to give the terminal addresses as arguments after the commands STM and RTM.

The terminal-addresses are stored as bits set into the variable ITRMAD file.

The following error-messages may be output:
a. MULTIPLEXER-ERROR –1 : Second multiplexer not connected.
b. MULTIPLEXER-ERROR –2 : Multiplexer not connected.

System option 1 may only be selected if there is a multiplexer AND a digital output card in the system. If there is no digital output card, selection is possible by manual setting of the switches on the multiplexer, but the system option 1 should not then be selected for output.

12. REMARKS ON THE COMPUTER HARDWARE

You will be aware that the computer hardware design is constantly changing, and we have taken advantage of this situation because of the use of microprocessors in our spectrometers.

The following hardware configurations are recommended:

1. **Philips**
   - *1.1. PW1790/11* — A P851 based computer system, with a dual floppy disc station for mass storage and program loading. The system has a full control panel, and is housed in a PW1735 cabinet. The PW1790/11 is the successor to the PW1790/10, which has a mini-panel.
     We will start using the P854 CPU as soon as the delivery situation permits.
   - *1.2. More powerful systems* based on the P800 line can only be quoted after Supply Centre approval.

2. **Digital Equipment Corporation (DEC)**
   The product line of DEC is being updated, and product types are being replaced. For the moment we recommend the following:
   - *2.1. PDT11 series.* This is an intelligent terminal with single density floppy discs. It is an attractive and cheap solution for a system using the RT11 software in applications where the customer uses our standard software, and does not want to make any software modifications. Current indications are that DEC will not supply the unit under any OEM agreements, and DEC are now starting to push their Mini Minc and Minc systems. The argument is that the customer can add his own software. We have the following comments:
     a. We have not yet tried our software with the Mini Minc/Minc systems, therefore, we cannot guarantee correct functioning of the complete system.
     b. Knowing the size of our own software programs, we can say that this configuration is too small to make any modifications.
     c. A customer can purchase a BASIC compiler from DEC which will allow him to write off-line programs.

     Note that our programs are written in FORTRAN, not in BASIC.

The VT 103 is an alternative sometimes proposed by DEC. Again a possiblity, but:
- our software has not been tested with such a system,
- a VT 103 configuration uses a VT 100 video display unit, so that a graphics terminal is not possible.

   - *2.2. PDP11/23.* A microprocessor based computer, which uses the PDP11/34 instruction set, and is configured around the sequential "Q-bus" (11/03 bus). This system can have a memory size up to 256 k byte. The PDP11/23 can support two firm discs (type RL01) and, therefore, becomes a good proposition for our RSX11-M package, which requires firm discs.
   - *2.3. PDP11/34.* A powerful computer system configured around the fast "Unibus". This system is field-proven. Because of internal competition from the PDP11/23, you may find that this system is competitive in price with a PDP11/23, and it has a short delivery time. You will also find that some customers already have a PDP11/34 system in-house, and they will want to connect our spectrometer to their own system.

NOTE: If you order your hardware from DEC be very careful that the correct interfaces and cables have been included.

3. **Hewlett Packard (HP)**
   - *3.1. HP9815.* A simple package is available which requires an HP9815 calculator to be connected as a slave to the second PW1715/00 interface in the spectrometer. The PW1400 is controlled from the main terminal. The package requires operator know-how on HP programming, and is similar to the demo-package we produced for the PW1410 AHP.
     Project code 9430 - 900 - 00901.
   - *3.2. HP85.* We anticipate having a software package for the HP85 available in the first or second quarter of 1981. We are still waiting for the release of the HP serial interface. This package would use the HP85 keyboard for spectrometer control, and will also process the incoming data. You will be advised as soon as possible on the progress and availability.

NOTE: The above are the only machines from HP which can be offered. If a customer insists on using different hardware, then he does so at his own risk.

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810408 SOFTWARE SURVEY NO. 2 XRA 164

PW 1400/00 and PW 1600/10

	Subject	Action required
		Already issued: PW 1400/00 – XRA 141, 142, 150, 153, 156, 157, 159, 161, 162 PW 1600/10 – XRA 157, 159, 161, 162, 163
1.	Software for XRF	
2.	PW 1490/40/41/45/50 and PW 1690/40/41/45/50 Functional differences between versions 3.1 and 3.0 of X14 (RT11-SJ) and 1.2 and 1.1 of X16 (RT11-SJ)	Replace software
3.	Extended description of changes implemented in X14D/X16D, versions 3.1/1.2	–
4.	PW 1490/75 Description of starting up the RSX11M, and the XRF software package.	New software
5.	Generation of the RSX11M operation monitor.	Customer to generate own monitor for additional features.

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1. SOFTWARE FOR XRF

1.1. PW 1490/.. Software package (X14)

CPU	Monitor	Medium	Version	Release date	Update number	Firm ware (μ-proc) prerequisites version	Remarks
/00 P851	FRTM	Single density disc	02.0	05-10-79	—	2.0	old
			02.1	10-03-80	9430 900 85001	2.0	old
			02.2	26-09-80	9430 900 85031	2.0	old
			02.3	30-01-81	9430 900 85111	2.0	new
/40 PDP11	RT11-SJ	Single density disc	03.0	15-08-80	9430 900 85021	2.0	old
			03.1	24-02-81	9430 900 85151	2.0	new
/41 PDP11	RT11-SJ	Double density disc	03.1	24-02-81	9430 900 85131	2.0	new
/45 PDP11	RT11-SJ	RL01 firm disc	03.0	09-10-80	—	2.0	old
			03.1	24-02-81	9430 900 85171	2.0	new
/50 PDT11	RT11-SJ	Single density disc	03.0	19-08-80	9430 900 85061	2.0	old
			03.1	24-02-81	9430 900 85181	2.0	new
/74* PDP11	RSX11-M	RK05 firm disc	—	—	—		
/75 PDP11	RSX11-M	RL01 firm disc	03.1	13-02-81	—	2.0	new
/76* PDP11	RSX11-M	RL02 firm disc	—	—	—		

1.2 PW 1690/.. Software package (X16)

C.P.U.	Monitor	Medium	Version	Release date	Update numbers	Firm ware (μ-proc) prerequisites version	Remarks
/00 P851	FRTM	Single density disc	02.0	23-05-80	—	2.1	old
			02.1	10-10-80	9430 900 85091	2.1	old
			02.2	15-01-81	9430 900 85121	2.1	new
/40 PDP11	RT11-SJ	Single density disc	01.1	15-08-80	9430 900 85041	2.1	old
			01.2	24-02-81	9430 900 85161	2.1	new
/41 PDP11	RT11-SJ	Double density disc	01.2	24-02-81	9430 900 85141	2.1	new
/45 PDP11	RT11-SJ	RL01 firm disc	01.2	24-02-81	—	2.1	new
/50 PDT11	RT11-SJ	Single density disc	01.1	05-08-80	9430 900 85071	2.1	old
			01.2	24-02-81	9430 900 85191	2.1	new
/74* PDP11	RSX-M	RK05 firm disc	—	—	—		
/75* PDP11	RSX-M	RL01 firm disc	—	—	—		
/76* PDP11	RSX-M	RL02 firm disc	—	—	—		

* Available second quarter 1981

2. FUNCTIONAL DIFFERENCES BETWEEN VERSION 3.1 AND 3.0 OF X14 (RT11-SJ) FUNCTIONAL DIFFERENCES BETWEEN VERSION 1.2 AND 1.1 OF X16 (RT11-SJ)

2.1. Version 4,0 of RT11 has been implemented. The files on the diskette are now longer. Therefore some modules have been deleted or changed:

a. COPY. COM is changed, X14. HED/X16. HED is not typed.
b. X14. HED/X16. HED is deleted.
c. A special monitor is generated, which is as short as possible on the disc, and has a midnight day rollover. There are two monitors in use:

   RT03SJ – for 50Hz and
   RT04SJ – for 60 Hz.

   For the PDT11 system diskette only the 60Hz monitor is present, as this monitor is valid for both 50Hz and 60 Hz systems.
d. In order to save the system parameter file and a full databank on the single density diskette (s), the RT11 utility PIP is deleted after the start up-file STARTS. COM has been eventually adapted (see 2.4. for this adaption). This utility is only required to delete, change and type files.
   The deletion of PIP. SAV can only be done on a copy of the original system diskettes, as otherwise PIP. SAV is lost forever!.
e. The new Fortran compiler and library (version 2.5) have been implemented in this version.

2.2. Three new output devices are introduced: T1, T2 and T3.

2.3. With some system parameter configurations using two devices that are not TT: for output, (e.g. RT and LP), and with simultaneously writing data to a disk file with the WDD command, the monitor can sometimes print the message "Error 30 – No room for buffers" because of lack of memory for assigning buffers for the input/output devices. In that case the start up file has to be changed. The line "SET USR NOSWAP" is changed to "SET USR SWAP".

2.4. The start- up file STARTS. COM contains the assign command for RT.
If this device is not in the system the following error message is generated by the RT11 monitor:
?KMON–F–illegal device RT: and the rest of the start up file will not be executed. The error message can be avoided by deleting the assignment for RT in the file STARTS. COM as follows:

Start the RT11 monitor from a diskette which contains PIP. SAV amd when the . is printed type:
COPY TT: STARTS. COM
Then type all lines of the original start-up file except the assignment for RT:
Finally change the SET USR NOSWAP line into SET USR SWAP and add any new lines if necessary.
<cntrlZ>
The last typed character is the cntrl Z to close the file.

2.5. The ASP command has been extended with the question for system options. The possible answers are 0 to delete all system options or one or more numbers in the range 1—16.

The system options available now are:

a. System option 3 (for PW 1600/10 only) to get a hard copy of concentrations output if a V.D.U. is used.

b. System option 4 (for PW 1400/00 and PW 1600/10) to print the question SAVE DATA in FILE ddi: xxxxxx.Cyy = YES : = , after a concentration output report.

2.6. The RT11 instal (INS) command is no longer required in RT11 version 4.

2.7. The AMT and MMT commands have been implemented to update the monitor buffers with the hardware monitor tray option (for PW 1600/10 only).

2.8. The file COPY. COM has been changed (see also point 2.1.).

2.9. The file STARTS. COM has been changed. The INSTALL command is not required in version 4.0 of RT11.

2.10. The system parameter file has been extended with system options (ASP, PSP COMMAND).

The following system options are defined:

1 Reserved
2 Reserved
3 Possibility to output hard copy if terminal is a V.D.U. (for PW 1600/10 only)
4 For question "SAVE DATA IN DISK FILE" after a concentration output
5 Reserved
6 Reserved

2.11. The module WRDATA for writing concentrations to a disc file has been replaced by module WRDISK.
Corrected errors:
The LUN used to print the disc file name will be closed, so the name is printed immediately after the concentration output report. If a new disc is mounted it is checked to see if there is already a file with the same name on the new disc.
Added features:
If system option 4 has been selected, there will be asked whether the data should be written to disc (only for normal concentrations if the WDD command has been given).
The file name will be derived from the sample identification if it is a normal concentration measurement and IDPNTR= 1—15.
The file is always closed at the return, unless it is a recalibration measurement.

2.12. The measurement times and recalibration indices are no longer lost after the ADF command.

2.13. The measurement times and recalibration indices are no longer lost after the ADS command.

3. EXTENDED DESCRIPTION OF CHANGES IMPLEMENTED IN X14D/X16D version 3.1/1.2.

Before making any changes on a diskette, make a copy of the original delivered diskette (see below) and store the original diskette in a safe place. Use the copy to tailor it to the operators wishes.
The copy procedure is as follows:

a. Place the original systems diskette in drive 0.
b. Place a fresh diskette in drive 1 it need not be initialised or formatted.
c. Boot drive 0 and type after the single point has appeared:
   @COPY. Answer the question.
d. After the process is ready (single point appears), store the original diskette in a safe place and place the copy from drive 1 in drive 0.
e. Boot drive 0.

3.1. RT11 version 4.0 and Fortran version 2.5 have been implemented in this version. The monitor RT03SJ.SYS on the diskette is a system generated monitor with 50Hz mains frequency support, and timer support for midnight date rollover; the monitor RT04SJ.SYS is a system generated monitor with 60Hz mains frequency support and timer support for midnight rollover.

For the PDT11 system, there is only the RT04SJ.SYS monitor for 60Hz on the diskette; this monitor is valid for both 50Hz and 60Hz systems.

If a double density diskette is booted, the 50Hz monitor will be booted automatically; to change over to the 60Hz monitor type the command @60Hz.

If the system diskette is single density, and the user wishes to have a full databank on that system diskette, the file PIP. SAV must be deleted from this diskette, but only after the above start-up file changes have been executed, as PIP will be removed from the diskette and the change of the start-up file uses this utility. Removal of PIP is necessary because insufficient space remains on the diskette for a full databank and the utility PIP.
The procedure for removing PIP. SAV is as follows:

a. Make a copy of the original system diskette (using @COPY)
b. Boot this diskette
c. Change, if necessary, the start-up file (see procedure below).
d. Type : DELETE PIP. SAV and answer the question
e. Type : SQUEEZE SY0: and answer the question.

It is advisable to have a second diskette where the PW 1400. SAV file has been removed and where the PIP. SAV file is present. This diskette can then be used for copying, renaming, deleting and typing of files.
If the operator wishes to make such a diskette, proceed as follows:

a. Make a copy of the original systems diskette.
b. Boot this diskette
c. Type : DELETE PW 1400. SAV/DELETE PW 1600. SAV and answer the question
d. Type : SQUEEZE SY0: and answer the question.

3.2. There are three new output devices introduced: T1, T2 and T3. These can be used for the 3 spare control units on a DLV11-J card, or for the optional cluster control unit on a PDT system. To use these devices they should be selected as output devices in the system parameters (ASP command).
If some of the drives T1, T2, T3 and/or RT are used by the operator in the XRF package (by assigning them in the system parameter file SYSPAR. DAT with the ASP command), change the start-up file by adding one or more of the assignments stated below (depending on which drivers are to be used):

ASS T1: 8
ASS T2: 9
ASS T3: 10

The RT-driver assignment (ASS RT: 4) is already present in the start-up file and can be omitted if the RT-driver is not in use.
If none of the drivers RT, T1, T2 or T3 are used, omit all ASS-lines from the file.

The renaming of the LP. SYS driver into drivers RT. SYS, T1. SYS, T2. SYS and T3. SYS is already done as follows (RT. SYS as example):

```
COPY/SYST LP. SYS, RT. SYS
SET RT VECTOR = 314
SET RT CSR = 175624
SET RT CR
SET RT LC
SET RT NOFORMO
SET RT NOFORM
```

The drivers T1 - T3 and RT have the following addresses:

DEV	CSR	VECTOR
T1	176504	304
T2	176514	314
T3	176524	324
RT	176524	310

These addresses can be changed with the RT11 SET command. e.g.

```
SET  RT  VECTOR = 314
SET  RT  CSR = 175624
```

If DL (V) 11 serial control units are used, the following addresses must be selected on the card(s):

RCSR = 176500 and vector 300 for T1
RCSR = 176510 and vector 310 for T2
RCSR = 176520 and vector 320 for T3
RCSR = 175620 and vector 310 for RT

NOTE 1 : RT and T2 cannot be used in the same system, because they use the same vectors.
NOTE 2 : If T1 is used with the above given vector, the vector of the DL (V) 11-E control unit for the spectrometer must be changed to e.g. 330. Do this as follows:
Switch the mains off and change the jumpers on the DL (V) 11-E card.
Start the RT11-monitor and delete the file SYSPAR. DAT from the diskette.
Start the spectrometer program, which will ask for the system parameters. Give the correct data for the DL (V) 11-E address and vector.

3.3. Because the monitor in core is longer, in some system parameter configurations using two devices that are not TT: for output (e.g. RT and LP), and with simultaneously writing data to a disk file with the WDD command, the user has to work with USR SWAP. This is not required for the PDT system, which has 2K additional core available.
If error 30 is given during running of the X14D/X16D software, the USR must be set to NOSWAP.
The change can be implemented in the start-up file if necessary by changing the line "SET USR NOSWAP" to "SET USR SWAP". See point 2.5. for the way to make this change.

E.g.
It may be necessary if a driver must be loaded for listing device 1 or 2, so TT it is not used. If USR is NOSWAP and listing device 1 is LP: one may see ERR 30 after the commands OFF followed by PSI or after WDD and SMX. If USR is NOSWAP and listing device 1 is TT: there are no problems with the commands ADF, ADC and ADS.
It is tested with a DY system diskette and monitor RT03SJ. SYS (Location 50 contains 135732 after . LOAD LP:). We see ERR 30 if the high limit in PW 1400. SAV/PW 1600. SAV is 23203 W ("132506) and we see no ERR 30 if the high limit is 23162 W ("132364).

3.4. (See description 2.4.).

3.5. The ASP command has been extended with the question for system options. The possible answers are 0 to delete all system options, or one or more numbers in the range 1-16.
The system options available now are:

a. System option 3 (for PW 1600/10 only) to get a hard copy of concentrations output if a V.D.U. is used. If system option 3 has been selected and the operators terminal is a V.D.U. (VT or GT), and listing device 1 is not TT, the system will display the concentrations on the terminal and then ask whether a hard copy must be made to listing device 1.

b. System option 4 to get the question SAVE DATA in file ddi:xxxxxx. Cyy = YES : = after a concentration output report.

****

Replacement of the start-up file STARTS. COM:

a. Type: COPY TT: STARTS. COM
b. Type all required lines for the new start-up file after the
c. Type: Control-Z

****

To type the contents of the original start-up file on the terminal, type: TYPE START. COM
The utility PIP. SAV must be present on the systems device.

****

The system is now ready to initialise and start the XRF package.
With RSX it is possible to start up the XRF package from any terminal connected to the system.
If the operator uses a terminal other than the one which was booted (so not TTO:), he must login according to the printout on that terminal (HEL SYSTEM/SYSTEM); the main terminal TTO: is already automatically logged.

To initialise the XRF package type XRF after the prompt.
At any time in this XRF file the answer to a question can be HELP, in which case a detailed description will be typed, clarifying the answer the system expects on the appropriate question (see example below).
The first question requests the device on which the XRF data files will be written - those files which are the result of the WDD command.
Proper devices are:

DLx: RL01 disc drive
DKx: RK05 disc drive
DXx: RX01 floppy drive
DYx: RX02 floppy drive

(in the above, x denotes a drive number)

If the XRF data files are written to the disc on which the system exists (DL0:), the operator can type in a single carriage return.
If some device other than DLx has been asked for, the system will look to see if this device is valid (supported by the system), and if the driver for that device is not loaded already it will load the driver.

NOTE 2 : Keep in mind that devices DY and DX cannot be used simultaneously, as the vector and external page addresses of both devices are the same.
The system will unload either DX or DY in the case where DY or DX has been asked for by the operator.

In case the device asked for not DL, the system will ask if an initialised medium has been inserted in the device. If not, this medium can be inserted and formatted without leaving the initialising procedure started by the command XRF (on line formatting).
A message DMO -- VOLUME NOT MOUNTED can be ignored.

NOTE 3 : The XRF data files will always be written under UIC 201,54 on the chosen device; this UIC will automatically be created on the device if not already present (so ignore the message UFD -- DIRECTORY ALREADY EXISTS).

After mounting the required device the system will ask for the terminal number of the remote terminal (the remote terminal is the one the operator assigns with RT using the ASP-command in the XRF package; see the PW 1400 Operation Manual).
Any terminal number that is supported to the system can be given.
If the operator types in a single carriage return, the terminal at which the XRF command has been given will be assigned as remote terminal also.

After having answered the last question, the system will make several assignments, look after the XRF package on the disc, instal these packages and types a list of features, typical for the answers given during the XRF command.

The XRF package can now be started with the command RUN PW 1400.

4. DESCRIPTION OF STARTING UP RSX11M AND THE XRF SOFTWARE PACKAGE

Switch on the equipment: DC ON (front panel)
System returns with:
001600 004000 004030 004200
Wait until LOAD lamp is lit.
(Disc drive needs time to spin up)
Insert SYSTEM disc if not already mounted.
Push LOAD — lamp goes out.
WAIT until READY 0 is lit. (SYSTEM disc is now on correct spinning speed)
Type DL.
System initializes itself and prints:

```
@DL

    RSX–11M V3.2 BL26  60K  MAPPED
> RED  DL:=SY:
> RED  DL:=LB:
> MOU  DL:RSXM26
> @DL: [ 1, 2 ] START UP
> * ENTER date and time ( dd-mm-yy hh:mm) [S] : 26-FEB-81 08:01
> TIM 26-FEB-81 08:01
> !
> ! ...WORKING...
> !
> * is this terminal a CRT ?[Y/N]  : N
> * What is the highest terminal number in this system [0]: 1
> !
> ! ...WORKING...
> !
>
Have a good morning
26-FEB-81 08:04 TTO:  LOGGED OFF
>

    RSX–11M BL26                    MULTI–USER SYSTEM

Good morning
26-FEB-81  08:04  LOGGED ON TERMINAL TTO:
```

The date and time-input will be requested, type the required data in the stated format, terminated with carriage return.
Next there will be asked if the main terminal is a CRT (cathode ray tube); if so, type Y followed by carriage return; if not, only type a carriage return. If the operator typed Y, the terminal will support the rubout feature if using the DELETE key.
Next the system asks what the highest terminal number in the system is; if more than one terminal TTO: is present, it sets the features for those terminals and broadcasts a message to the other terminal on how to login with the system.
At the end of the start-up command file a single prompt > . will be typed.

NOTE 1 : The command HELP can be typed in after the start-up file has been terminated. By doing so the operator can print some features that the system incorporates on his terminal. The HELP command can be given at any time, unless the XRF package is running.

4.1. ENCOUNTERING A PROBLEM IN THE XRF-PACKAGE (NOT IN STANDARD DEC RSX11M SOFTWARE MODULES)

If the operator encounters a problem or error in the XRF software package, he should include in the software problem report as much of the output that shows what commands are given to cause the problem.
Keep in mind that it is possible that a command which seemed to be executed correctly beforehand can cause the problems later.

NOTE 4 : The user should send not only the above-mentioned output, but also the output generated with the PRO command.
To generate this output, which includes all the features and conditions in the system at the time the error occured, the user first must leave the XRF package by giving the END command (if the XRF package was not terminated by the RSX system itself), and then after the DEC prompt > he should give the PRO command. This command must be given on a terminal that selects printing on paper.

4.2. SWITCHING OFF PROCEDURE

If the XRF package is not terminated, type END and wait until the prompt > appears; then type BYE.
If the terminal was not the main terminal TT0:, the operator can logout the main terminal also with the command BYE.

```
* END

*** SPECTROMETER OFF
> BYE
>
HAVE A GOOD MORNING
DMO -- TT1:          DISMOUNTED FROM DY0:
05-MAR-81 10:55 TT1:  LOGGED OFF
>
DMO -- TT1:          DISMOUNTED FROM DY0:     *** FINAL DISMOUNT ***
DMO -- TT1:          DISMOUNTED FROM KL0:

>
```

4.3. EXAMPLE OF STARTING UP THE XRF PACKAGE WITH DATA FILES ON DL

```
> XRF
> ;STARTING UP THE XRF -- PACKAGE
> ;
> ; If any question is not clear, type HELP as answer to that question
> ;
> * DEVICE FOR YOUR XRF DATA FILES IF NOT DL0 (XXX:):? [ S ] :
UFD -- DIRECTORY ALREADY EXISTS
> * TERMINAL NUMBER OF THE REMOTE TERMINAL IF NOT 0 ? [ S ] :
> !
> ! ...WORKING...
> !
;
;
;    ****************************************
;
;    ***** SOFTWARE PACKAGE          : X14D-003.1 RSX11M
;    *****
;    ***** MAIN PACKAGE              :PW 1400. TSK;1
```

```
;    ***** CREATION DATE                : 06-FEB-81 14:53
;    ***** I/O PACKAGE                  : IOPAGE. TSK; 3
;    ***** CREATION DATE                : 27-NOV-80 11:18
;    ***** STARTED AT                   : 05-FEB-81 11:54:42
;    ***** ON DEVICE/UIC                : DL0: [ 201,54 ]
;    ***** XRF DATA FILES ON            : DL0: [ 201,54 ]
;    ***** REMOTE TERMINAL              : TT0:
;
;    ****************************************
> ;
> ; ***** TO CHANGE LAST TWO FEATURES OF ABOVE LIST, TYPE: > XRF
> ;
> ; ***** TO RUN THE XRF SOFTWARE PACKAGE' TYPE: > RUN PW 1400
> @> EOF >
>
>
```

4.4. EXAMPLE OF STARTING UP THE XRF PACKAGE WITH A DATA FILES NOT ON DL

```
> XRF
> ; STARTING UP THE XRF – PACKAGE
> ;
> ; If any question is not clear, type HELP as answer to that question
> ;
> *DEVICE FOR YOUR XRF DATA FILES IF NOT DL0 (XXX:) : ? [ S ] : DY0:
> ;
> ; ***** DEVICE DRIVER FOR DY:  NOT LOADED
> ;
> *MUST DRIVER FOR DY: BE LOADED NOW? [ S ] : Y
> !
> ! ...LOADING THE DRIVER...
> !
UNL -- DRIVER NOT LOADED
> *IS THERE A FORMATTED MEDIUM PRESENT IN DY0: (Y/N)? [ S ] : N
> *INSERT A MEDIUM TO BE FORMATTED IN DY0:; READY (Y/N)?[ S ] :Y
DMO -- VOLUME NOT MOUNTED DY0:
> *WHAT IS THE VOLUME NAME ( 12 CHARS MAX.)?[ S ] : TEST X14D
> *WHAT DENSITY (DOUBLE, SINGLE)? [ S ] : DOUBLE
> ALL DY0:
>INS $FMT
> !
> ! ...FORMATTING ON DY0:...
> !

** WARNING – DATA WILL BE LOST ON DY0: **

CONTINUE? [ Y OR N ] : Y

START FORMATTING

START VERIFICATION

OPERATION COMPLETE

> !
> ! ...INITIALISING DY0:...
> !
INI -- NO BAD BLOCK DATA FOUND
```

```
> *IS UNIT DY0: READY TO BE MOUNTED [ S ]  : Y
> *TERMINAL NUMBER OF THE REMOTE TERMINAL IF NOT 0? [ S ]  : 1
> !
> ! ...WORKING...
> !
;
;
;   ****************************************
;
;   ***** SOFTWARE PACKAGE          : X14D–003. 1 RSX11M
;   *****
;   ***** MAIN PACKAGE              : PW 1400. TSK; 1
;   *****CREATION DATE              : 06–FEB–81 14:53
;   ***** I/O PACKAGE               : IOPAGE. TSK; 3
;   ***** CREATION DATE             : 27–NOV–80 11:18
;   ***** STARTED AT                : 05–MAR–81 10:52:45
;   ***** ON DEVICE/UIC             : DL0: [ 201,54 ]
;   ***** XRF DATA FILES ON         : DY0: [ 201,54 ]
;   ***** REMOTE TERMINAL           : TT1:
;
;   ****************************************
> ;
> ; ***** TO CHANGE LAST TWO FEATURES OF ABOVE LIST, TYPE: > XRF
> ;
> ;  ***** TO RUN THE XRF SOFTWARE PACKAGE, TYPE : > RUN PW 1400
> @ < EOF >
>
>
```

4.5. EXAMPLE OF STARTING UP THE XRF PACKAGE WITH DATA FILES NOT ON DL DEVICE DRIVER ALREADY LOADED AND FORMATTED MEDIUM IN DEVICE.

```
> XRF
> ; STARTING UP THE XRF–PACKAGE
> ;
> ; If any question is not clear, type HELP as answer to that question
> ;
> *DEVICE FOR YOUR XRF DATA FILES IS NOT DL0 (XXX:) :?  [ S ] : DY0:
> *IS THERE A FORMATTED MEDIUM PRESENT IN DY0: (Y/N)? [ S ] : Y
> *IS UNIT DY0: READY TO BE MOUNTED [ S ]  : Y
UFD –– DIRECTORY ALREADY EXISTS
> *TERMINAL NUMBER OF THE REMOTE TERMINAL IF NOT 0?  [ S ] : 1
> !
> ! ...WORKING...
> !
;
;
;   ****************************************
;
;   ***** SOFTWARE PACKAGE          : X14D–003.1 RSX11M
;   *****
;   ***** MAIN PACKAGE              : PW 1400. TSK; 1
;   ***** CREATION DATE             : 06–FEB–81 14:53
;   ***** I/O PACKAGE               : IOPAGE. TSK; 3
;   ***** CREATION DATE             : 27–NOV–80 11:18
;   ***** STARTED AT                : 05–MAR–81 10:54:13
;   ***** ON DEVICE/UIC             : DL0: [ 201,54 ]
;   ***** XRF DATA FILES ON         : DY0: [ 201,54 ]
;   ***** REMOTE TERMINAL           : TT1:
;
```

```
;   ****************************************
> ;
> ; ***** TO CHANGE LAST TWO FEATURES OF ABOVE LIST, TYPE :> XRF
> ;
> ; ***** TO RUN THE XRF SOFTWARE PACKAGE, TYPE:> RUN PW 1400
> @<ECF>
>
>
```

4.6. EXAMPLE OF TERMINATING XRF PACKAGE AND LOGOUT

First properly terminate the XRF package by the command END.
Then logout with command BYE (on all terminals if you want to remove the disc).
To remove the disc from the DL drive, release the LOAD button on the disc drive and wait until the LOAD lamp is lit. Then remove the disc and eventually switch off the computer.

DIFFERENCES BETWEEN XRF PACKAGE ON RT11 and RSX11

a. A single slash terminates a command, so do not use the / in text strings (e.g. in CP–list headings or sample identifications).
b. The /M, /S, /T commands from XRF–RT11 are replaced by the CTR–L, CTRL–H and the CTRL–T keys respectively.
c. Do not terminate the four commands mentioned above with a carriage return.
d. Purge your data banks and system parameter files at the end of a session, using the command PUR after the RSX prompt > appears.
   If you do not purge your files the disc can become filled up, leaving no room for any more data files and thus producing error messages if running the XRF package.
e. If your computer system has only 64K of memory and the XRF package has been started, no additional DEC utilities can be started due to space problems. If a user starts such a utility it will not be moved to memory until the XRF package, which is non-check pointable, is removed from the memory (i.e. is terminated with the END command).

5. GENERATING A RSX11M OPERATION MONITOR

The following procedure is shown AS AN EXAMPLE ONLY so that users with a DEC PDP11 computer can generate their own program (executive) on the system disc, to include features not present in the X14 (version 3.1.) software.
This executive has been created on AUTOPATCH LEVEL B.

If the user wants to use additional features, which are not included in the executive, he must generate the new system, whereby the following features must be included in new executive:

TERMINAL ATTACH FUNCTION
CINT $ DIRECTIVE
AST SUPPORT
FULL DUPLEX TERMINAL DRIVER
MINIMAL 64K WORDS OF MEMORY – MAPPED

The DL11E should not be included in the system generation.
The DL11E vector- and external page addresses should not be used by any peripheral in the generated system.
In particular, note the Target configuration on page 1-4.
For convenience the following procedure is reproduced from a computer readout.

[illegible]

```
      Leave DL0:  at WRITE PROTECTED.
   j. Place the MAPSRC system generation disc in DL0:  and wait till it has become ready.
   k. Place a fresh disc in DL1:  (need not to be initialised nor formatted;  the data present on this disc  will
      be destroyed by the copying process), wait till it has become ready
   l. Type after the prompt :
      DSCS8 DL1:=DL0:
      and wait till the copying process is ready (another DSCS8: is typed)
   m. remove the system generation disc MAPSRC from DL0:  and store it away
   n. leave the copy of MAPSRC in DL1:
   o. Place the copy of RSXM26 in DL0:  and wait till it has become ready.
   p. set DL0:  to WRITE ENABLED

   Now copies have been made from the original system generation discs;  in the following pages these discs  will
   be referred to as RSXM26 and MAPSRC.

2. Boot DL0:

     022001 000001 000510 001274
     @DL

     RSX-11M V3.2 BL26   60K    MAPPED
      RED DL1:=SY:
      RED DL:=LB:
      MOU DL:RSXM26
      @DL:[1,2]STARTUP
     >* PLEASE ENTER TIME AND DATE (HR:MN DD-MMM-YY) [S:] 11:53 16-DEC-80
     >TIM 11:53 16-DEC-80
     >* ENTER LINE WIDTH OF THIS TERMINAL [D R:132.]: 80.
     >SET /BUF=TI:80.
     >ACS SY:/BLKS=512.
     >;
     >; NOTE - The Baseline INDirect must be replaced by BIGIND with
     ;        a priority of 10. for SYSGEN.
     >;
      ;  ie  >REM ...AT.
     >;       >INS $BIGIND/PRI=10.
     >;
      ?  EOF
      REM  ...AT.
     >INS $BIGIND/PRI=10.
     INS -- WARNING - PRIVILEGED TASK OVERMAPS I/O PAGE
     >REM MAC
      REM INB
     INS $BIGMAC/INC=50000
     INS -- PARTITION PAR14K NOT IN SYSTEM, DEFAULTING TO GEN
     >INS $BIGINB/INC=50000
     INS -- PARTITION PAR14K NOT IN SYSTEM, DEFAULTING TO GEN
     >SET /UIC
     UIC=[200,200]
     >@SYSGEN
     >;
     >; RSX-11M Ver. 3.2 BL26 System Generation 3.2.3 done on 16-DEC-80 at 11:54:06
```



```
     >;
     >; Copyright (C) 1979 Digital Equipment Corporation,Maynard Mass.
     >;
     >; RL01 distribution kit
     >;
      *  1. Inhibit MCR command lines (Type .ESC/ for explanation)? [Y/N]:N
     >*  2. Have you made a copy of the distribution kit? [Y/N]:Y
      *  3. Use saved or canned answer file for input responses [Y/N]:N
     >* 10. Save responses (i.e.; create SYSSAVED.DAT)? [Y/N]:Y
     >* 11. UIC for SYSSAVED files if not [200,200]  [S]: <cr>
     >* 12. UIC for SYSGEN command files if not [200,200] [S]: <cr>
      * 13. Clean up files from previous GENs? [Y/N]:Y
     >* 14. Device, when ready, for Executive sources (ddu:)  [S]: DL1:
      ;
      MOU DL1:MAPSRC
      ASN DL1:=LB:
      ;
      SET /UIC=[1,1]
      PIP [1,2]RSXBLD.CMD;*/DE/NM,SYSPAR;*
      PIP [1,24]RSXBLD.CMD;*/DE/NM,TTDRVBLD;*,SYSPAR;*
      PIP [1,50]SYSVMR.CMD;*/DE/NM,[1,54]LYSVMR;*
      PIP [11,20]*.OBJ;*/DE/NM,*.UDC;*,*.ICR;*,*.IDS;*,*.PCS;*
      PIP [11,20]RSXASM.CMD;*/DE/NM,RSXDRVASM;*,RSXBLD;*
      PIP [11,24]*.OBJ;*/DE/NM,*.UDC;*,*.ICR;*,*.IDS;*,*.TTY;*,*.PCS;*
      PIP [11,24]RSXASM.CMD;*/DE/NM,RSXDRVASM;*,RSXBLD;*
      PIP [11,10]SYSTB.MAC;*/DE/NM,ICTAB;*,RSXMC;*,[200,200]SGNPARM.CMD;*
      PIP [11,10]RSXASM.CMD;*/DE/NM,RSXDRVASM;*,RSXBLD;*
      PIP /FR

     DL0: HAS 5128. BLOCKS FREE, 5112. BLOCKS USED OUT OF 10240.
     LARGEST CONTIGUOUS SPACE = 3976. BLOCKS

      SET /UIC=[11,10]
      ;
      ; Target configuration
      ;
      *  1. Processor (e.g.; 11/34, LSI-11) [S R:5-6]: 11/34
     >*  2. Does processor have a switch register? [Y/N]:N
      *  3. Generating RSX-11S? [Y/N]:N
      *  4. Memory size (in K-word blocks) [D R:16.-124.]: 64.
      *  5. Mapped? [Y/N]:Y
      *  6. Any K-series laboratory devices? [Y/N]:N
      *  7. Floating point processor (FP-11) present? [Y/N]:N
      * 10. If using KW11-P as system clock: number of intrs./sec  [D R:0.-1000.]:
      * 11. Line frequency:  A- 60 Hz    B- 50 Hz   [D: 'A'] [S]: B
      * 12. KW11-W Watchdog timer support? [Y/N]:N
      * 13. Memory parity support? [Y/N]:N
      * 15. Highest interrupt vector (If 0 will be computed) [D R:0-774]:  <cr>
     >;     For device configuration: '*' Prints device table, '.' Terminates
     >;     Enter devices and number of controllers for devices which require drivers
      * 16. Devices [S]: NL,TT,DL,DK,LP,DY,DX
     >* 16. DEVICES [S]: .
```

```
;*
;* Processor:11/34   Memory Size:64K,Mapped   System:RSX-11M
;*
;* Host configuration
;*
;*  1. Are you running SYSGEN standalone (on the baseline system)? [Y/N]:Y
;*  2. Is a line printer available? [Y/N]:N
;*  4. Does the listing/map device have at least 120 columns? [Y/N]:N
;*  5. Assembly listings device (ddu:) [D: *NL*] [S]: <cr>
;*  6. Map device for Executive and device drivers (ddu:) [D: SY:] [S]: <cr>
;*
;* EOS * Do you want to: <CR>-continue R-repeat section E-exit P-pause [S]: <cr>
;*
;* Executive Options
;*
;*     Answer Y(ES) if the following support is desired
;*
;*  2. FILES-11 ACP ? [Y/N]:Y
;*  3. RMS record locking and placement control? [Y/N]:N
;*  4. Non-resident tasks (task loader)? [Y/N]:Y
;*  5. Loadable task-loader? [Y/N]:Y
;*  6. Memory management (PLAS) directives? [Y/N]:N
;*     Address checking support will be included
;*     I/O rundown support will be included
;* 11. Multi-user protection? [Y/N]:Y
;* 12. ANSI Magtape ACP? [Y/N]:N
;* 13. On-line formatting (FMT) or on-line user-mode diagnostics? [Y/N]:N
;* 14. Loadable device drivers? [Y/N]:Y
;* 15. Should the default for all applicable drivers be loadable? [Y/N]:Y
;* 16. AST and cancel selective MARKTIMEs? [Y/N]:Y
;* 17. Task termination and device not ready messages (TKTN)? [Y/N]:N
;* 18. Power fail recovery? [Y/N]:N
;* 19. Install, request, and remove on exit? [Y/N]:Y
;* 20. Large (20K) Executive? [Y/N]:N
;* 21. Logical device assignment? [Y/N]:Y
;* 22. Logging of device errors and timeouts? [Y/N]:N
;* 23. Logging of undefined interrupts? [Y/N]:N
;* 25. Do you intend to include a user-written driver? [Y/N]:N
;* 28. Disk writecheck? [Y/N]:N
;* 29. Executive Debugging Tool (XDT)? [Y/N]:N
;* 31. Industrial network or DECnet? [Y/N]:N
;* 32. Queue manager and queued print spooler? [Y/N]:N
;* 33. Group global event flags? [Y/N]:N
;*     For directives: '*' Prints table, '.' Terminates inquiry, '%' Gets all
;* 34. Enter code for directives [S]: %.
;*     SGN -- WARNING -- CPU does not have switch register
;*         -- Get sense switch directive not included
;* 35. Number of pre-allocated QIO packets [D R:0.-15. D:5.]: <cr>
;* 36. Size of data transfer vector in words [D R:5.-33. D:33.]: <cr>
;* 37. Round-robin scheduling interval in ticks [D R:0.-100. D:5.]: <cr>
;* 38. Highest priority class for consideration [D R:1.-249. D:150.]: <cr>
;* 39. Lowest priority class for consideration [D R:1.-150. D:1.]: <cr>
```



```
;* 40. Executive level disk swapping interval [D R:0.-5000. D:30.]: <cr>
;* 41. Swapping priority [D R:1.-20. D:5.]: <cr>
;* 42. Size of dynamic storage region (POOL) in words [D R:256.-16384. D:1024.]: <cr>
;* 45. System crash register and stack dump device CSR [O R:0-177700 D:1775641]: <cr>
;* 46. Checkpointing:              A- Yes    B- With system ckpnt. file    [S]: B
;* 47. System cntrld partitions: A- Yes    B- With auto compaction (SHF) [S]: B
;* 48. Dump analysis:              A- PANIC  B- Crash (CDA)                [S]: <cr>
;*
;* Terminal driver options
;*
;*  1. Terminal driver desired (A/B/C/D, * prints table) [S]: C
;*  2. Unsolicited input timeout value in seconds [D R:0.-2540. D:120.]: <cr>
;*
;*     Answer Y(ES) if the following support is desired
;*
;*  5. Task checkpointable during terminal input? [Y/N]:Y
;*  6. Unsolicited input character AST? [Y/N]:Y
;*     Breakthrough write support will be included
;*     CTRL/R support will be included
;* 10. Escape sequence handling? [Y/N]:Y
;* 11. Get multiple characteristics? [Y/N]:Y
;* 12. Set multiple characteristics? [Y/N]:Y
;* 13. Get terminal driver options? [Y/N]:Y
;* 17. Read after prompt? [Y/N]:Y
;* 20. CRT rubout support? [Y/N]:Y
;* 25. Hardware unrecoverable input error notification? [Y/N]:Y
;* 26. Device independent cursor positioning? [Y/N]:Y
;*
;* EOS * Do you want to: <CR>-continue R-repeat section E-exit P-pause [S]: <cr>
;*
;*     Thinking ...
;
; End of Executive option generation at 12:02:34 on 16-DEC-80
;
; Peripheral configuration
;
;     Parameters appearing in square brackets "[...]" can only be
;     specified for the first controller of a particular device.
;     Parameters appearing in parentheses "(...)" only need be specified
;     if the indicated option is present on the target system.
;
;     The default for loadable drivers has been set to *TRUE*.
;     To override this setting enter R (resident) as the first parameter
;     for the first controller of the specified device.
;
; A/D and Laboratory devices: None specified
;
; Interprocessor communication devices: None specified
;
; Unit record devices: LP
;
; Enter [L/R,] vector, CSR, printer type
```

```
;             (,[KMC timeout count <0=no KMC>, KMC vector, KMC CSR]) for:
;
;* 16. LP controller 0 [D: 200,177514,LA180-0,300,160130] [S]: <cr>
;
; Disks: DK, DL, DX, DY
;
; Enter [L/R,] vector, CSR, highest unit number <0 to 7> for:
;
;*  6. DK controller 0 [D: 220,177404]             [S]: ,,0
;
; Enter [L/R,] vector, CSR, number of drives for:
;
;*  3. DL controller 0 [D: 160,174400]             [S]: ,,2
;* 53. Contr 0 unit 0. is an RL01/RL02 [D: RL01]   [S]: <cr>
;* 53. Contr 0 unit 1. is an RL01/RL02 [D: RL01]   [S]: <cr>
;
;*  3. DX controller 0 [D: 264,177170]             [S]: ,,2
;
;*  3. DY controller 0 [D: 264,177170]             [S]: ,,2
;* 58. Contr 0 unit 0. is SINGLE/DOUBLE density    [S]: SINGLE
;* 58. Contr 0 unit 1. is SINGLE/DOUBLE density    [S]: SINGLE
;
; Tapes: None specified
;
; Non-physical (pseudo) devices: CO, TT, NL, TI, CL, LB, SY
;
; Enter num. DL11's <ZL>, num. DH11's, num. DZ11's, num. DJ11's for:
;
* 20. The terminal driver  [D: 1,0,0,0]           [S]: 2,0,1,0
;
; Enter vector, CSR, E=DL11-E modem support/NO=no for:
;
* 21. ZL controller 0 [D: 60,177560,NO]           [S]: <cr>
* 21. ZL controller 1 [D: ,,NO]                   [S]: 310,175620
;
; Enter vector, CSR, highest line number <0 to 7> [, answer speed] for:
;
;* 24. DZ controller 0 [D: ,,,0]                  [S]: 320,160010,7,0
SET /UIC=[1,24] ! Creating TTDRVBLD.CMD
SET /UIC=[11,10]
;
* EOS * Do you want to: <CR>-continue R-repeat section E-exit P-pause [S]: <cr
;
;
; End of interrupt vector area has been set to 400
;
;
; Create Executive build files
;
PIP RSXMC.MAC=LB:RSXMC0.MAC/AP
;
; Assemble the Executive
```



```
;
PIP [11,24]/NV=RSXASM.CMD,RSXDRVASM.CMD
PIP RSXASM.CMD;0/DE,RSXDRVASM;0
;
*  1. Do you wish to edit any of the Executive files? [Y/N]:N
;
;
* EOS * Do you want to: <CR>-continue R-repeat section E-exit P-pause [S]: <cr
;
;SET /TEABREAK=TI: Start of Executive assembly at 12:15:15 on 16-DEC-80
SET /UIC=[11,24]
MAC @RSXASM
;SET /NOTEABREAK=TI: Executive assembly ended at 12:35:22 on 16-DEC-80
;
;* EOX * Did the Executive assemble correctly? [Y/N]:Y
;
;SET /TEABREAK=TI: Start of device drivers assembly at 12:35:27 on 16-DEC-80
SET /UIC=[11,24]
MAC @RSXDRVASM
;SET /NOTEABREAK=TI: Device drivers assembly ended at 12:49:57 on 16-DEC-80
;
;* EOX * Did the device drivers assemble correctly? [Y/N]:Y
;
;
; Prepare for task building
;
PIP RSX.OBS=*.OBJ
PIP *.OBJ;*/DE/NM
PIP RSX11M.OBJ/RE=RSX.OBS
PIP TTDRV.OBJ=*.TTY
PIP *.TTY;*/DE/NM
SET /UIC=[1,24]
PIP /NV=[11,10]RSXBLD.CMD
;
* EOX * Do you want to: <CR>-continue R-repeat section E-exit P-pause [S]: <cr
;
;
; End of SYSGEN Phase I at 12:52:30 on 16-DEC-80
;      -- To continue type: @[200,200]SYSGEN2
;
SET /UIC=[200,200]
@ "EOF"
SYSGEN2
;
; RSX-11M Version  3.2 System Generation Phase II started 16-DEC-80 at 12:52:40
;
; Copyright (C) 1979 Digital Equipment Corporation, Maynard Mass.
;
*  1. In what UIC is SGNPARM.CMD if not [200,200] [S]: <cr
;
; RL01 distribution kit SYSGEN versions 3.2.3. / 2:3.2.2d  for RSX11M BL26
;
```

```
        ; Continuation from SYSGEN Phase I done on 16-DEC-80 at 12:52:22
        ;
        *  3. Expanded comments desired for SYSGEN Phase II? [Y/N]:Y
        *  4. Is SYSGEN still running stand-alone? [Y/N]:Y
        ;
        ;     If running a single RL01 kit enter either 'NO' or 'NONE' in reponse
        ;     to the next question if the [1,24] files have not been copied
        ;     onto the RSXM26 disk.
        ;
        ;     Note that it will first be necessary to delete [11,10]*.MAC; however
        ;     before you do this first copy RSXMC.MAC and SYSTB.MAC to some other
        ;     UIC.
        ;
        *  5. If not in DL1: enter object files device when ready (ddu:) [S]: <cr>
       ;
       MOU DL1:MAPSRC
       MOU -- OTHER VOLUME MOUNTED - DL1:
       ASN DL1:=LB:
       ASN S:=DK:
       PIP /FR

       DL0: HAS 4897. BLOCKS FREE, 5343 BLOCKS USED OUT OF 10240.
       LARGEST CONTIGUOUS SPACE = 3976. BLOCKS

        *  6. Have you already built the libraries, the Exec, and the loadable drivers?
        ;
        ; Start of Executive and driver build phase at 12:53:37 on 16-DEC-80
        ;
        *  8. Create ANSLIB to support Big-buffering? [Y/N]:N
        INS $LBR
        SET /UIC=[1,1]
        SET /UIC=[1,24]
        PIP RSX11M.OLB;*/DE/NM,TTDRV;*
        LBR RSX11M/CR:80.:640.:256.=[11,24]RSX11M.OBJ
        LBR TTDRV/CR:52.:256.:64.=[11,24]TTDRV.OBJ
        PIP LB:/NV=LB:MCR.OLB
        LBR LB:MCR/RP=LB:MCRTTFD
       MODULE 'SDSOV' REPLACED

       MODULE 'SETOV' REPLACED

       MODULE 'SPROV' REPLACED

        ;
        ; Taskbuild the Executive and the terminal driver at 12:55:17 on 16-DEC-80
        ;
        PIP [1,34]*.*;*/DE/NM
        TKB @RSXBLD
       ;
       * EOX * Did the Executive build succesfully? [Y/N]:Y
       ;
       SET /UIC=[1,54]
```



```
        PIP LB:/NV=RSX11M.STB
        SET /UIC=[1,24]
        TKB @TTDRVBLD
       ;
        * EOX * Did the terminal driver build succesfully? [Y/N]:Y
       ;
        * 10. List Executive map? [Y/N]:Y
        ;
        ; Build Loadable drivers
        ;
        *  6. Device for driver's maps [D: NL:] [S]: <cr
        *  9. Build all selected loadable drivers into DRVPAR? [Y/N]: N
       ;
       ;
       ; When all drivers are built, strike carriage return
        ;
       * 10. Driver 2-character device mnemonic [S]: DL
       * 11. Driver partition name [D: DRVPAR]  [S]: GEN
        TKB @[200,200]DLDRVBLD
       PIP [200,200]DLDRVBLD.CMD;*/DE
       PIP [1,54]DLDRV.STB/TR
       * 10. Driver 2-character device mnemonic [S]: DK
       * 11. Driver partition name [D: DRVPAR]  [S]: GEN
       TKB @[200,200]DKDRVBLD
        PIP [200,200]DKDRVBLD.CMD;*/DE
       PIP [1,54]DKDRV.STB/TR
       * 10. Driver 2-character device mnemonic [S]: LP
       * 11. Driver partition name [D: DRVPAR]  [S]: GEN
        TKB @[200,200]LPDRVBLD
        PIP [200,200]LPDRVBLD.CMD;*/DE
       PIP [1,54]LPDRV.STB/TR
       * 10. Driver 2-character device mnemonic [S]: DY
       * 11. Driver partition name [D: DRVPAR]  [S]: GEN
        TKB @[200,200]DYDRVBLD
        PIP [200,200]DYDRVBLD.CMD;*/DE
        PIP [1,54]DYDRV.STB/TR
        * 10. Driver 2-character device mnemonic [S]: DX
        * 11. Driver partition name [D: DRVPAR]  [S]: GEN
        TKB @[200,200]DXDRVBLD
        PIP [200,200]DXDRVBLD.CMD;*/DE
        PIP [1,54]DXDRV.STB/TR
        * 10. Driver 2-character device mnemonic [S]: <cr
        ;
        ; End of library, Executive and driver build phase at 13:08:04 on 16-DEC-80
       ;
       ; Start task building privileged tasks at 13:08:07 on 16-DEC-80
       ;
       * 11. FCP desired  (Type 'ESC' for explanation)  [D: MIDDLE] [S]: <cr>
        * 14. Build the task FMD? [Y/N]:N
        * 15. Build RMDEMO? [Y/N]:N
        * 16. Build the non-queue manager print spooler? [Y/N]:Y
        ;
```

```
;
;     Note that the following task-builds will be executed for your system:
;
;       BOOBLD    DMOBLD    FCPMD1BLD INDBLD    INIBLD    INSBLD    MCRMUBLD
;       MOUBLD    SAVBLD    UFDBLD    LOABLD    UNLBLD    SHFBLD    PRTBLD
;       ACNTBLD   BYEBLD    HELBLD    BROBLD    SHUTUPBLD ACSBLD
;
;* 17. Edit any privileged task build files? [Y/NJ:N
;
;     For the dual RK05 or RL01 distribution kits, running standalone,
;     you may direct the task builder maps to the line printer, or to
;     printer, or another disk of the same type as your kit.  Note that
;     the maps will not fit on the distribution disks for the above.
;
;     For other distribution kits, you may specify the line printer,
;     the distribution kit disk (SY0) or a second disk of the same type.
;
;     For all online SYSGENs, you may specify any disk with al least
;     1400 free blocks.  Note that SYSGEN will not load the driver for
;     this disk.
;
;* 18. Map device for privileged tasks (ddu:) [D: NL:] [S]: <cr>
;
ASN NL:=MP:
ASN LB:=SY:
ASN =LB:
ASN =SY:
ASN DL1:=SY:
ASN DL0:=LB:
TKB @BOOBLD
TKB @DMOBLD
TKB @FCPMD1BLD
TKB @INDBLD    ! GENERATING SMALL INDIRECT
TKB @INIBLD
TKB @INSBLD
TKB @MCRMUBLD
TKB @MOUBLD
TKB @SAVBLD
TKB @UFDBLD
TKB @LOABLD
TKB @UNLBLD
TKB @SHFBLD
TKB @PRTBLD
TKB @ACNTBLD
TKB @BYEBLD
TKB @HELBLD
TKB @BROBLD
TKB @SHUTUPBLD
TKB @ACSBLD
;
* EOX * Did the privileged tasks build succesfully? [Y/NJ:Y
;
; End of privileged task builds at 13:31:59 on 16-DEC-80
```



```
;
ASN LB:=SY:
ASN =LB:
ASN =SY:
ASN DL0:=SY:
ASN DL1:=LB:
SET /UIC=[1,54]
PIP /FR

DL0: HAS 3785. BLOCKS FREE, 6455. BLOCKS USED OUT OF 10240.
LARGEST CONTIGUOUS SPACE = 3752. BLOCKS

;
;     SGN -- SYSGEN will now pause to allow you to create your
;            RSX11M.SYS file using the following example. Ideally
;            your system it should occupy the same number of blocks
;            as indicated in the example
;
;            PIP RSX11M.SYS/NV/CO/BL:258.=RSX11M.TSK

AT. -- PAUSING. TO CONTINUE TYPE 'RES ...AT.'

>PIP RSX11M.SYS/NV/CO/BL:258.=RSX11M.TSK
>RES ...AT.

AT. -- CONTINUING

;
;     Your target system is now ready to set up partitions and install
;     the required tasks.  SYSGEN has created a file SYSVMR.CMD; edit
;     this command file to do the following:
;
;     1) Extend pool space to base of first partition
;     2) Set up your partitions, particularly your device partitions
;     3) Install the privileged tasks you just build
;     4) Load any loadable drivers that you want resident
;        in the system image.  If the terminal and/or system
;        disk drivers are loadable, they must be loaded using VMR.
;
;     When VMR prompts ENTER FILENAME> respond with @SYSVMR
>;
>;     Note that for mapped systems the SYSVMR file will typically
>;     produce a valid system image without editing; for unmapped
>;     systems no such claim is made.  It is, however, our best guess.
>;     Note that on unmapped systems no driver partitions are created
>;     by SYSGEN.  You must edit them in yourself.
>;
>;
>* 19. Edit SYSVMR.CMD? [Y/NJ:Y
>;
>EDI SYSVMR.CMD
[00044 LINES READ IN]
```

```
[PAGE   1]
*PL TTPAR
SET /MAIN=TTPAR:*:400:TASK
*DP
LOA TT:
*DP
SET /MAIN=DRVPAR:*:*:SYS
*DP
LOA DK:
*DP
LOA DL:
*DP
LOA DX:
*DP
LOA DY:
*DP
LOA LP:
*DP
SET /TOP=DRVPAR:-*
*DP
SET /MAIN=SYSPAR:*:100:TASK
*
SET /MAIN=FCPPAR:*:240:SYS
*
SET /MAIN=GEN:*:*:SYS
*I
LOA TT:/PAR=GEN
LOA DK:/PAR=GEN
LOA DL:/PAR=GEN
LOA DX:/PAR=GEN
LOA LP:/PAR=GEN

*
INS FCPMD1      ! INSTALL FILE SYSTEM
*DP
INS ACS         ! INSTALL ALLOCATE CHECKPOINT FILE
*N -10
*
FIX ...LDR
*
SET /MAIN=SYSPAR:*:100:TASK
*
SET /MAIN=FCPPAR:*:240:SYS
*I
INS FCPMD1      ! INSTALL FILE SYSTEM

*B
*PL *
SET /POOL=*
*C /*/600
SET /POOL=600
*ED
```



```
[EXIT]

>INS SY:$BOO/-1
 INS $VMR/-1
 ASN SY:=LB:
 VMR
ENTER FILENAME: @SYSVMR
VMR -- PARTITION SPLPAR NOT IN SYSTEM, DEFAULTING TO GEN
POOL=600:4092.:04092.
LDRPAR 057744 060000 002400 MAIN TASK
SYSPAR 057454 062400 010000 MAIN TASK
FCPPAR 057420 072400 024000 MAIN SYS
GEN    057300 116400 261400 MAIN SYS
       057244 116400 016700 SUB  DRIVER - TT:
       056730 135300 000600 SUB  DRIVER - DK:
       056640 136100 001500 SUB  DRIVER - DL:
       056550 137600 002300 SUB  DRIVER - DY:
       056460 142100 001000 SUB  DRIVER - LP:
...LDR 11A    057660 LDRPAR 248. 002400 LB0:-00013035 FIXED
...DMO 23.00  056170 GEN    160. 040000 LB0:-00013204
MCR... 02.01  055500 SYSPAR 160. 010000 LB0:-00013752
...MOU 22.15  055244 GEN    160. 040000 LB0:-00013352
...MCR 01     055010 GEN    160. 020000 LB0:-00013776
F11ACP V0320  057334 FCPPAR 149. 024000 LB0:-00013245
SHF... 04     055074 SYSPAR 105. 010000 LB0:-00013421
...INS 04     055734 GEN    100. 040000 LB0:-00013317
...SAV 04.22  055160 GEN    100. 040000 LB0:-00014206
...UFD V0410  054724 GEN    100. 040000 LB0:-00013402
PRT... 08.04  055650 GEN     70. 010000 LB0:-00014247
...AT. 04.25  056104 GEN     65. 040000 LB0:-00013554
...INI 20.02  056020 GEN     60. 040000 LB0:-00013432
...ACS 01     056340 GEN     50. 040000 LB0:-00013715
...BOO 03.4   056254 GEN     50. 040000 LB0:-00013156
...LOA 03.3   055564 GEN     50. 040000 LB0:-00013660
...HEL 02     055414 GEN     50. 040000 LB0:-00014302
...BYE 02.5   055330 GEN     50. 004000 LB0:-00013474
...UNL 02.8   054640 GEN     50. 040000 LB0:-00014114
LP0:    LOADED
DK0:    LOADED
DL0:    LOADED
DL1:    LOADED
DX0:    UNLOADED
DX1:    UNLOADED
DY0:    LOADED
DY1:    LOADED
TT0:    LOADED
TT1:    LOADED
TT2:    LOADED
TT3:    LOADED
TT4:    LOADED
TT5:    LOADED
TT6:    LOADED
```

```
TT7:    LOADED
TT10:   LOADED
TT11:   LOADED
NL0:
TI0:
CO0:  TI0:
CL0:  TT0:
LB0:  DK0:
SY0:  DK0:
VMR>Z

 ;
 ;     When the indirect file exits, boot in your target system,
 ;     set the date and time, and save the system with a bootstrap.
 ;     When your system reboots itself, purge the old task files.
 ;
 ; E.G.
 ;       BOO RSX11M
 ;       TIM 9:00:00 13-JAN-56
 ;      >SAV /WB
 ;
 ;      RSX11M V03.2 BL26   64K  MAPPED
 ;       RED DL0:=SY:
 ;      >RED DL0:=LB:
 ;      >MOU DL0:RSXM26
 ;      @[1,2]STARTUP
 ;      >* Enter date and time ( dd-mm-yy hh:mm ) [S]:
 ;      TIM 9:00:04 13-JAN-56
 ;      >@ <EOF>
 ;       SET /UIC=[1,54]
 ;      >RUN $PIP
 ;      PIP>*.*/PU
 ;      PIP>Z
 ;
 ;
>;      Don't forget to create accounts after saving your system
>REM LBR
>ASN =LB:
>;
>; End of SYSGEN Phase II at 13:40:32 on 16-DEC-80
 ;
>@ <EOF>
```


The PW1400 task generation process uses the followins UICs :

```
[201,24]   objects, task-build files
[201,34]   map files
[201,54]   task files
[201,14]   for user-written of user-modified source modules

[1,1]      default object library PHILIB.OLB.
           This special library will be used with task buildins the PW1400 task and  contains  the  followins
           items :
           SYSLIB.OLB
           FOROTS.OLB
           IREADW
           ITTOUR
           IWRITW
           PURGE
           PUTSTR
```

In case a new version of the RSX11M software (after current version 3.2) will become available, the default library PHILIB.OLB should be renewed with the aid of the utility LBR (see Utilities Manual); the above standins special routines IREADW,ITTOUR,IWRITW,PURGE and PUTSTR should be included in the new library.

For task buildins the PW1400 task, two task-buildins files are present under UIC [201,24]:
XR14HPBLD.CMD and XR14HP.ODL

The XR14HP.ODL file is an overlay description language file, XR14HPBLD.CMD is the indirect command file used with the TKB command.

The contents of these two files will follow :

```
; COMMAND FILE XR14HPBLD.CMD FOR X14D V3.1
; DATE : 19-NOV-80
;
[201,54]PW1400/PR:0,[201,34]PW1400/-SP/-SH=[201,24]XR14HP/MP
ASG=SY:1
ASG=LP:6
ASG=TI:5
ASG=TT1:4
MAXBUF=512
STACK=100
FMTBUF=80
ACTFIL=3
//


;            FILE XR14HP.ODL FOR X14D VERSION 3.1
;
     .ROOT MAIN-LIB-*(A,B,C,D,E)
```

```
SOFTWARE-DESCRIPTION X14D-SOFTWARE FOR PDP11 - RSX11M                    PAGE 1-17
Generation PW1400 task


;
;
MAIN:        .FCTR M1-M2-M3-M4-M5-M6-M7-M8-M9
;
;
M1:  .FCTR PW14HPRSX-KBCOMPRSX-ISTOP-KBINPT-INITPR-IENTER
M2:  .FCTR KBINPCRSX-CVNAME-CARRET-CRLF-IGNAME-LOOKUP
M3:  .FCTR KBNAME-IGCHAR-IASSIRRSX-KBCHAR-KBINTG-KBREAL
M4:  .FCTR ERROR-INVALD-KBINCR-KBINCI-KBICHK-KBRCHK
M5:  .FCTR LFETCH-LDBWDBRSX-KBNAMCRSX-IUPINP-UPINIT-PRNTUP
M6:  .FCTR UPCOM1RSX-IWAITR-UPERR-INTASC-IVDUCHRSX-PRTUP2
M7:  .FCTR LOOKFFRSX-GTDATE-NEWFLTRSX-NEWFILRSX-KBFILN
M8:  .FCTR NOYESF-SPAWNCRSX
M9:  .FCTR SEQ-[1,1]PHILIB/LB:$SHORT
;
;
A:   .FCTR HT1-(HT21,HT22)
B:   .FCTR AN1-(AN21,AN22,AN23,AN24)
C:   .FCTR AS1-(AS21,AS22,AS23)
D:   .FCTR RG1-(RG21,RG22,RG23)
E:   .FCTR UP1
;
;
HT1: .FCTR HWTESTRSX-CSTPRGRSX-AUTPLTRSX-RWCOM-KBDCTA
HT21:        .FCTR PHDHPRRSX-ENDCOMRSX-PLSHPRRSX-PLOTHP-CHITOL
HT22:        .FCTR CSTHPRRSX
;
AN1: .FCTR ANALYSRSX-DINTAS-ANACOM-RATIO-MICROP-ICHECK-IDINPT
;
AN21:        .FCTR SMACOM-SMXCOM-PRINT-LIMCHK-STATER
AN22:        .FCTR MONUPDRSX-MANINP-MANLCIRSX-NORMAC-BACKGR-AN22CN
AN22CN:      .FCTR LOVCOR-MANCOM-ASINDARSX-INTRAT-MODULI
AN23:        .FCTR WRDISKRSX-WDDCOM-HERZOG
AN24:        .FCTR IRECALRSX-RECALCRSX-JOBCOMRSX
;
;
AS1: .FCTR ASSEMBRSX-MOVDWN-MOVUP-MOVDELRSX-INCRDBRSX-AS1CON
AS1CON:      .FCTR LDBCOM-PMBCOM-PNMCOM-RFBCOMRSX-DPBCOMRSX-AS2CON
AS2CON:      .FCTR UPCOMD-PCPCOM-PLFCOM
;
AS21:        .FCTR ACPCOMRSX-PLLCOM-ALLCOMRSX-AMBCOMRSX-PMMCOM
AS22:        .FCTR ASPPSPRSX-ST14HPRSX-IGTMSK-PRMASK-KBDCTA-AMSCOMRSX
AS23:        .FCTR ALPCOMRSX-PMSCOM-AMLCOMRSX-PMLCOM-PRCCOM-AS23CN
AS23CN:      .FCTR ANMCOMRSX-ARCDRCRSX
;
;
RG1: .FCTR REGRESRSX
;
RG21:        .FCTR SRRCOMRSX-MOVDELRSX-INCRDBRSX-SRICOMRSX-RG21CN
RG21CN:      .FCTR ISRIDKRSX-NREDSK-MOVUP
RG22:        .FCTR PRLHP-SRACOM-PRTDEA-SOLVE
RG23:        .FCTR PLTHPRRSX-AUTPLTRSX
```

```
SOFTWARE-DESCRIPTION X14D-SOFTWARE FOR PDP11 - RSX11M                    PAGE 1-18
Generation PW1400 task


;
;
UP1: .FCTR UPDATERSX-OPFCOMRSX-ADCDLCRSX-DLSCOM-CVDATE-ADSCOM-UP1CON
UP1CON:      .FCTR ADFCOMRSX-PCSCOM-ACDCOMRSX-UPRCOM-CCICOMRSX-PJFCOM
;
;
LIB: .FCTR [1,1]PHILIB/DL
;
;
     .END
```

The task-building (linking-) process itself will be processed if the operator types the command L14; the indirect command file that is started then, initialises the system for the task-build of the X14D software, whereby the operator can decide whether to delete the old X14D task or not.
For the outlay of this indirect command file, called TKBX14D.CMD, see chapter 9.

The task-building process may take some 20 minutes using the BIGTKB on a PDP 11/34.

If some user-written sources are added to the task-building, they must be compiled without sequencenumbers, without array vectoring and without optimalisation for speed, e.g.: >FOR [201,24]filename,filename=[201,14]filename/NOSN/NOVA/-OP:SPD , this for reducing the space requirements of a routine.
The new sources must be located under UIC 201,14.

SOFTWARE-DESCRIPTION X14D-SOFTWARE FOR PDP11 - RSX11M
Command file STARTUP.CMD


```
.; Indirect command file STARTUP.CMD
.;
.; This command file sets the conditions for RSX11 environment
.;
.;
     .ENABLE SUBSTITUTION
.;
.; Ask proper time from operator
.;
     .ASKS TIM Enter date and time ( dd-mmm-yy hh:mm )
     TIM 'TIM'
     !
     ! ...WORKING...
     !
     .ENABLE QUIET
.;
.; Prepare checkpointfile on DL0:
.; This file is used for saving temporarily checkpointed files
.;
     ACS DL:/BLKS=500.
.;
.; Unload non-used drivers
.; After having given the command >X14 and the driver
.; must be used by the PW1400 task, the task will
.; automatically ask for the correct driver if it is
.; not already loaded
.;
     .IFLOA DY: UNL DY:
     .IFLOA DX: UNL DX:
     .IFLOA DK: UNL DK:
.;
.; Install privileged tasks
.; TDX is the catch all task, which tries to perform commands unknown
.; to MCR (such as the PROBLEM command)
.;
     INS $PIP
     INS $FOR/INC=40000
     INS $BIGMAC/PAR=GEN/INC=50000
     INS $BIGTKB/PAR=GEN
     INS $EDI
     INS $BRO
     INS $TDX
     SET /MAXEXT=30.K
.;
.; INSTALL SERIAL DESPOOLER
.;
     SET /PUB=TT1:
     .IFNINS PRT... .GOTO 90
     REM PRT...
.90: INS $PRT/PAR=GEN
     REA PRT... 3 LP:
.;
```

SOFTWARE-DESCRIPTION X14D-SOFTWARE FOR PDP11 - RSX11M
Command file STARTUP.CMD


```
.; SET COMMANDS FOR TT0:
.;
     SET /BUF=TI:200.
     SET /LOWER=TT0:
     SET /TYPEAHEAD=TT0:
     SET /WRAP=TT0:
     SET /FORMFEED=TT0:
     .ASK ANSWR IS THIS TERMINAL A CRT
     .IFF ANSWR .GOTO NOCRT
     SET /CRT=TT0:
.NOCRT:
.;
.; ASK FOR HIGHEST TERMINALNUMBER PRESENT IN SYSTEM
.; (THIS MUST BE ASKED FOR SET UP THESE TERMINALS)
.;
     .ASKN NUMBER WHAT IS THE HIGHEST TERMINALNUMBER IN THIS SYSTEM
     .DISABLE QUIET
     !
     ! ...WORKING...
     !
     .ENABLE QUIET
     .IF NUMBER < 1 .GOTO NORT
     .SETN TERNUM 1
.;
.; SET COMMANDS FOR TTxx:
.;
.NEXTR:
     SET /TYPEAHEAD=TT'TERNUM':
     SET /WRAP=TT'TERNUM':
     SET /BUF=TT'TERNUM':200.
     SET /LINES=TT'TERNUM':57.
     SET /LOWER=TT'TERNUM':
     SET /FORMFEED=TT'TERNUM':
     .IF TERNUM = 1 .GOTO NEXT
     SET /SPEED=TT'TERNUM':9600:9600
.NEXT:
     .INC TERNUM
     .IF TERNUM <= NUMBER .GOTO NEXTR
.;
.; END OF STARTUP
.;
     .SETN TERNUM 1
.NEXBR:
     BRO TT'TERNUM': TO ENTER THE SYSTEM, TYPE >HEL SYSTEM/SYSTEM
     .INC TERNUM
     .IF TERNUM <= NUMBER .GOTO NEXBR
.NORT:
     BYE
     HEL SYSTEM/SYSTEM
```

```
.; Indirect command file SETUPXRF.
.;
.; Used for setting correct features for the XRF software package
.;
      .ENABLE SUBSTITUTION
      ; STARTING UP THE XRF - PACKAGE
      ,
      ; If any question is not clear, type HELP as answer on that question
      ;
.;
.; Abort any active PW1400 or IOPAGE task; this can occur if the
.; task was not properly terminated the foregoing time
.;
      .ENABLE QUIET
      .IFACT PW1400 ABO PW1400
      .IFACT IOPAGE ABO IOPAGE
.;
.; Remove the old PW1400 and IOPAGE task
.;
      .IFINS PW1400 REM PW1400
      .IFINS IOPAGE REM IOPAGE
.;
.; Install the new PW1400 and IOPAGE task
.;
      INS   SYDISK:'<SYUNIT>':[201,54]PW1400
      INS   SYDISK:'<SYUNIT>':[201,54]IOPAGE
.;
.; Check if the PW1400 and IOPAGE task have been found on the
.; system disk
.;
      .IFNINS PW1400 .GOTO NOPW14
      .IFINS IOPAGE .GOTO BEGIN0
.;
.; One or both tasks not found in [201,54]; type warning that
.; the XRF package cannot be executed
.;
.NOPW14:
      .DISABLE QUIET
      ;
      ;
      ; ***** PW1400 SOFTWARE PACKAGE CANNOT BE FOUND ON
      ; ***** DISC '<SYDISK>''<SYUNIT>'[201,54]
      ;
      , **** CORRECT THE ERROR AND TYPE AGAIN: XRF
      ;
      .STOP
.;
.; Assign proper device as system-device
.;
      .ENABLE QUIET
.BEGIN0:
      ASN '<SYDISK>''<SYUNIT>':=SY0:
```



```
.;
.; Ask which device must be used as data-files device
.; if only <cr> given, the systemdevice will be the data-files device
.;
.BEGIN:
      .DISABLE QUIET
      .ASKS FILDEV DEVICE FOR YOUR XRF DATA FILES IF NOT '<SYDISK>''<SYUNIT>':?
      .IF FILDEV NE 'HELP' .GOTO BEGIN1
      ,
      ; There is no need to save the files, originating from the WDD command
      ; of the XRF package, on the same device where the XRF package
      ; resides ('<SYDISK>''<SYUNIT>':).
      ; The user can direct this files to another device, whereby the device
      ; driver must be present on the systemdevice at [1,54]. If the device
      ; driver cannot be found on the systemdevice, a warning will be typed
      ; and the operator can choose a correct device.
      ; The correct UIC under which the data files will be written
      ; ([201,54]) will be created on the medium by this program.
      ; If this UIC is already present, it will not be destroyed,
      ; but a warning will be typed, which can be ignored
      ;
      .GOTO BEGIN
.BEGIN1:
      .IF FILDEV EQ "" .SETS FILDEV "'<SYDISK>'"+"'<SYUNIT>'"+":"
.;
.; Test if typed in code from operator is correct device specification
.;
      .TEST FILDEV
      .IF <STRLEN> GT 4 .GOTO ERROR
      .SETS TEST FILDEV[:STRLEN>:<STRLEN>]
      .IF TEST NE ":" .SETS FILDEV FILDEV+":"
      .TEST FILDEV
      .IF <STRLEN> LE 4 .GOTO CONT
.;
.; The device specification was incorrect; try again after message
.;
.ERROR:
      ; ***** DEVICE SPECIFICATION 'FILDEV' INCORRECT
      .GOTO BEGIN
.;
.; The device specification was correct; test if driver for that
.; device has already been loaded
.;
.CONT:
      .SETS DEV FILDEV[1:2]+":"
      .IFLOA 'DEV' .GOTO NEXT
.;
.; The device driver is not loaded yet; ask if it must be loaded
.; automatically
.;
      ;
      ; ***** DEVICE DRIVER FOR 'DEV' NOT LOADED
```

```
        ;
.CONT7:
        .ASKS DRIVER MUST DRIVER FOR 'DEV' BE LOADED NOW?
        .IF DRIVER EQ "" .SETS DRIVER "N"
        .IF DRIVER NE "HELP" .GOTO CONT8
        ;
        ; The operator asked for a data-files device ('FILDEV'), for which
        ; the driver is not already loaded.
        ; By answering "Y" on the question, the device driver 'DEV' will be
        ; searched on the system device under UIC [1,54] and loaded.
        ; If the device driver 'DEV' cannot be found, a warning will be typed
        ; and this question will be repeated.
        ; By answering "N" on the foregoing question, you must load the
        ; driver yourself, e.g. from a foreign medium, not already mounted
        ; by the system.
        ;
        .GOTO CONT7
.CONT8:
        .DISABLE QUIET
        !
        ! ...LOADING THE DRIVER...
        !
        .ENABLE QUIET
        .SETS DRIV DRIVER[1:1]
        .IF DRIV EQ "Y" .GOTO NEXT1
        .DISABLE QUIET
        ;
        ; ***** LOAD THE CORRECT DRIVER AND THEN START THIS SEQUENCE
        ; ***** WITH @XRF AGAIN
        .STOP
        .ENABLE QUIET
.;
.; Driver must be loaded automatically; test if driver is present
.; on system device in UIC 1,54 (the .STB file must be present).
.;
.NEXT1:
        .ENABLE QUIET
        PIP TEMP.TMP;77777/DE/NM
        .WAIT PIP
        PIP TEMP.TMP;77777=[1,54]*.STB/LI/BR
        .WAIT PIP
        .DISABLE QUIET
        .SETS DEVNME FILDEV[1:2]+"DRV.STB"
        .OPENR TEMP.TMP;77777
.CLEA:
        .READ RECORD
        .IFT <EOF> .GOTO OUT
        .IF <FILERR> NE 1 .GOTO OUT
        .TEST RECORD
        .IF <STRLEN> <= 2 .GOTO CLEA
        .SETS A RECORD[3;<STRLEN>]
        .PARSE A ";" NAME VERS
```



```
        .IF NAME EQ DEVNME .GOTO OUT2
        .GOTO CLEA
.;
.; The driver cannot be found on the systemdevice; try again with
.; other driver
.;
.OUT:       .CLOSE  0
        ;
        ; ***** THIS DRIVER IS NOT PRESENT ON '<SYDISK>''<SYUNIT>':
        ;
        .GOTO BEGIN
.;
.; Finally load the driver
.;
.OUT2:
        .CLOSE  0
        .ENABLE QUIET
        PIP TEMP.TMP;77777/DE/NM
        LOA 'DEV'
        .DISABLE QUIET
.;
.; If the data-files device is not the system-device, try to
.; mount this device after acknowledge of operator that device is ready
.;
.NEXT:
        .SETS TEM "'<SYDISK>''<SYUNIT>'"+":"
        .IF FILDEV EQ TEM .GOTO NEXT2
.FORT0:
        .ASKS FORTST IS THERE A FORMATTED MEDIUM PRESENT IN 'FILDEV'?
        .IF FORTST EQ "" .SETS FORTST "N"
        .IF FORTST NE "HELP" .GOTO FORT1
        ;
        ; If no formatted medium is present in 'FILDEV', answering "N"
        ; on this question gives the possibility to format a medium on
        ; 'FILDEV' without leaving the startup procedure for XRF.
        ;
        .GOTO FORT0
.FORT1:
        .IF FORTST EQ "Y" .GOTO FORT3
.FORT2:
        .ASKS FORMAT INSERT A MEDIUM TO BE FORMATTED IN 'FILDEV'; READY?
        .IF FORMAT EQ "" .SETS FORMAT "N"
        .IF FORMAT NE "HELP" .GOTO FORM0
        ;
        ; A formatted medium must be present  lateron in the chosen
        ; device 'FILDEV', because the UIC [201,54] must be initialised
        ; on the medium, if it is not already present.
        ; If no formatted medium is present for 'FILDEV', this question
        ; gives the possibility to format a medium on 'FILDEV' without
        ; leaving this startup procedure for XRF.
        ; If a medium must be formatted, insert a medium in 'FILDEV'
        ; and give the answer "Y".
```

```
      .GOTO FORT2
.FORM0:
      .IF FORMAT EQ 'N' .GOTO FORT0
.AGAIN:
      .ENABLE QUIET
      DMO 'FILDEV'/DEV
      .DISABLE QUIET
      .SETS DEN 'SINGLE'
      .SETS VOL FILDEV[1:2]
      .SETS VOL1 FILDEV[1:3]
      .IF VOL1 EQ 'DL0' .GOTO ERROR
      .IF VOL EQ 'SY' .GOTO ERROR
.FORM0:
      .ASKS VOLNAM WHAT IS THE VOLUMENAME (12 CHARS MAX.)?
      .IF VOLNAM NE 'HELP' .GOTO FORM1
      ;
      ; The medium to format can be given a volumename, which will be printed
      ; with the mount command and by which an unprivilesed user can mount the
      ; device.
      ; The volumename HELP is not possible.
      ;
      .GOTO FORM0
.FORM1:
      .SETS DEV FILDEV[1:2]
      .SETS DENS DEN
      .IF DEV NE 'DY' .GOTO CONT
.FORM2:
      .ASKS DENS WHAT DENSITY (DOUBLE,SINGLE)?
      .IF DENS NE 'HELP' .GOTO FORM3
      ;
      ; The user can format his device in double or single density format
      ; depending on the fact if an RX02 is present or not. Single density
      ; mediums can be read in RX02 units as well as double density mediums
      ;
      .GOTO FORM2
.FORM3:
      .IF DENS EQ '' .SETS DENS DEN
      .IF DENS EQ 'SINGLE' .GOTO CONT1
      .IF DENS EQ 'DOUBLE' .GOTO CONT1
      .GOTO FORM2
.CONT:
      .ASK ANSWER ***** 'FILDEV'/ Initialise ? are you sure
      .IFF ANSWER .GOTO EXIT
.CONT1:
      ALL 'FILDEV'
      .IF DEV NE 'DY' .GOTO CONT2
      .IFNINS FMT INS $FMT
      .DISABLE QUIET
      '
      ! ...FORMATTING ON 'FILDEV'...
      '
```



```
      .ENABLE QUIET
      FMT 'FILDEV'/DENS='DENS'/VE
.CONT2:
      .DISABLE QUIET
      '
      ! ...INITIALISING DY0:...
      '
      .ENABLE QUIET
      .IF DEV EQ 'DY' .GOTO FLOPPY
      .IF DEV NE 'DX' .GOTO FIRM
.FLOPPY:
      INI 'FILDEV''VOLNAM'/INDX=BEG
      .DISABLE QUIET
      .GOTO EXIT
.FIRM:
      .ENABLE QUIET
      INI 'FILDEV''VOLNAM'
      .DISABLE QUIET
      .GOTO EXIT
.ERROR:
      ; ********** The systemdisc 'FILDEV' cannot be initialised!!! ***********
      .GOTO AGAIN
.ERROR2:
      ; ********** 'FILDEV' UNKNOWN ************
      .GOTO AGAIN
.EXIT:
      .DISABLE QUIET
      .GOTO FORT0
.FORT3:
.NEXT0:
      .ASKS MOUNT IS UNIT 'FILDEV' READY TO BE MOUNTED
      .IF MOUNT EQ '' .SETS MOUNT 'N'
      .IF MOUNT NE 'HELP' .GOTO NEXT8
      ;
      ; The operator has asked for a data files device 'DEV' that is
      ; not the system device '<SYDISK>''<SYUNIT>':.
      ; 'FILDEV' must be mounted and assigned as SY1 before any files
      ; can be written to it by the XRF software.
      ; Furthermore an UIC [201,54] must be created on 'FILDEV' if it
      ; is not already created before.
      ;
      .GOTO NEXT0
.NEXT8:
      .IF MOUNT EQ 'Y' .GOTO NEXT2
      .GOTO NEXT0
.NEXT2:
      .ENABLE QUIET
      MOU 'FILDEV'/OVR
      ASN 'FILDEV'=SY1:
.;
.; Create the UIC [201,54] on the data-files device if not already
.; present on this device.
```

```
.;
.; If already present, the files in this UIC will not be
.; erased
.;
      UFD 'FILDEV'[201,54]
      .DISABLE QUIET
.;
.; Ask which terminal should be used as remote terminal
.;
.CONT0:
      .ASKS NUMTRM TERMINAL NUMBER OF THE REMOTE TERMINAL IF NOT 0?
      .IF NUMTRM EQ "" .SETS NUMTRM "0"
      .IF NUMTRM NE "HELP" .GOTO CNT1
      ;
      ; If the user directs the output to a second, remote terminal (by
      ; assigning the output terminal to RT  with the ASP command of
      ; the XRF software ), he must type in the terminalnumber of the
      ; remote terminal.
      ; In case no remote terminal is used or if TT0: is the remote
      ; terminal, just type in a <cr>.
      ;
      .GOTO CONT0
.CNT1:
      !
      ! ...WORKING...
      !
.;
.; Assign the remote terminal to the correct terminalnumber
.;
      .ENABLE QUIET
      REA PW1400 4 TT'NUMTRM':
      .DISABLE QUIET
.;
.; Try to find the name, version and creation date of the PW1400
.; and IOPAGE tasks to save them in the PW1400.DAT file (used at
.; starting-up time and with the command >PROBLEM
.;
      .ENABLE QUIET
      PIP TEMP.TMP;77777=[201,54]PW1400.TSK,IOPAGE/LI
      .DISABLE QUIET
      .WAIT PIP
      .OPENR TEMP.TMP;77777
      .SETF PW1400
      .SETF IOPAGE
.CLEAN:
      .READ RECORD
      .IFT <EOF> .GOTO END
      .IF <FILERR> NE 1 .GOTO ERRFIL
      .TEST RECORD
      .IF <STRLEN> <= 2 .GOTO CLEAN
      .SETS A RECORD[3:<STRLEN>]
      .PARSE A ".;" NAME TYPE VERS
```



```
      .IFT PW1400 .GOTO SECND
      .IF NAME NE "PW1400" .GOTO SECND
      .IF TYPE NE "TSK" .GOTO CLEAN
      .SETS NAM1 NAME
      .SETS TYP1 TYPE
      .SETS VER1 VERS
      .SETT PW1400
      .READ RECORD
      .TEST RECORD
      .SETS B RECORD[14:<STRLEN>]
.SECND:
      .IFT IOPAGE .GOTO CLEAN
      .IF NAME NE "IOPAGE" .GOTO CLEAN
      .SETS NAM2 NAME
      .SETS TYP2 TYPE
      .SETS VER2 VERS
      .SETT IOPAGE
      .READ RECORD
      .TEST RECORD
      .SETS C RECORD[14:<STRLEN>]
      .GOTO END
.ERRFIL:
.;
.; Check if the file PW1400.DAT is already present on the systemdevice
.;
.END:
      .CLOSE  0
      .SETF PW1400
      .ENABLE QUIET
      PIP TEMP.TMP;77777/DE/NM
      .WAIT PIP
      PIP TEMP.TMP;77777='<SYDISK>''<SYUNIT>':[201,54]PW1400.DAT;77777/LI/BR
      .DISABLE QUIET
      .OPENR  0 TEMP.TMP;77777
.CLEN:
      .READ RECORD
      .IFT <EOF> .GOTO THEND
      .IF <FILERR> NE 1 .GOTO THEND
      .TEST RECORD
      .IF <STRLEN> <= 2 .GOTO CLEN
      .SETS A RECORD[3:<STRLEN>]
      .PARSE A ";" NAME VERS
      .IF NAME EQ "PW1400.DAT" .GOTO FOUND
      .GOTO CLEN
.;
.; This file was not present; catch the version of the XRF software
.; from the ST14HPRSX.FTN source-file from [201,14]
.;
.THEND:
      .CLOSE  0
      .OPENR '<SYDISK>''<SYUNIT>':[201,14]ST14HPRSX.FTN
.STRT:
```

```
      .READ RECORD
      .IFT .EOF> .GOTO STRT2
      .IF <FILERR> NE 1 .GOTO STRT3
      .TEST RECORD
      .SETS A RECORD[1:3]
      .IF A NE '10   ' .GOTO STRT
      .SETS SOFVER RECORD[14.:30.]
      .GOTO STRT4
.STRT3:
.STRT2:
.;
.; The file PW1400.DAT has been found; save the software version
.; from this file for later use
.;
.FOUND:
      .CLOSE  0
      .OPENR '<SYDISK>''<SYUNIT ':[201,54]PW1400.DAT;77777
      .READ MES1
      .READ MES1
      .READ MES2
      .READ MES1
      .READ MES3
      .SETT PW1400
.STRT4:
      .CLOSE  0
      .ENABLE QUIET
      SET /UIC=[201,54]
      .DISABLE QUIET
.;
.; Save features of start-up procedure in PW1400.DAT
.;
      .ENABLE QUIET
      PIP '<SYDISK>''<SYUNIT>':[201,54]PW1400.DAT;77777/DE/NM
      .DISABLE QUIET
      .WAIT PIP
      .OPEN '<SYDISK>''<SYUNIT>':[201,54]PW1400.DAT;77777
      .IFT PW1400 .GOTO STRT5
      .SETS MES1 "!"
      .SETS MES2 "! **********************************************"
      .SETS MES3 "! ***** SOFTWARE PACKAGE  : '+''SOFVER''
.STRT5:
      .SETS MES4 "! *****"
      .SETS MES5 "! ***** MAIN PACKAGE      : "+''NAM1''+"."+''TYP1''+";"+''VER1''"
      .SETS MES6 "! ***** CREATION DATE     : "+''B''"
      .SETS MES7 "! ***** I/O PACKAGE       : "+''NAM2''+"."+''TYP2''+";"+''VER2''"
      .SETS MES8 "! ***** CREATION DATE     : "+''C''"
      .SETS MES9 "! ***** STARTED AT        : '+'' DATE ''+' '+'  TIME..''"
      .SETS MES10 "! ***** ON DEVICE/UIC     : "+''<SYDISK>''+''<SYUNIT>''+":[201,54]"
      .SETS MES11 "! ***** XRF DATA FILES ON : "+''FILDEV''+"[201,54]"
      .SETS MES12 "! ***** REMOTE TERMINAL   : "+"TT"+''NUMTRM''+":"
      .DATA  0 'MES1'
      .DATA  0 'MES1'
```



```
      .DATA  0 'MES2'
      .DATA  0 'MES1'
      .DATA  0 'MES3'
      .DATA  0 'MES4'
      .DATA  0 'MES5'
      .DATA  0 'MES6'
      .DATA  0 'MES7'
      .DATA  0 'MES8'
      .DATA  0 'MES9'
      .DATA  0 'MES10'
      .DATA  0 'MES11'
      .DATA  0 'MES12'
      .DATA  0 'MES1'
      .DATA  0 'MES2'
      .CLOSE  0
.;
.; Print this startup features on the terminal
.;
      .ENABLE QUIET
      PIP TI:='<SYDISK>''<SYUNIT>':[201,54]PW1400.DAT;77777
      .DISABLE QUIET
.;
.; Give some information on how to change foregoing information and
.; on how to start the XRF package
.;
      ;
      ; ***** TO CHANGE LAST TWO FEATURES OF ABOVE LIST, TYPE: >XRF
      ;
      ; ***** TO RUN THE XRF SOFTWARE PACKAGE, TYPE : >RUN PW1400
      ;
```

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equipment for science and industry

810602 SOFTWARE SURVEY NO. 3. XRA167

PW1400/00 AND PW1600/10

Subject	Action required
	Already issued: PW1400/00 - XRA141, 142, 150, 153, 156, 157, 159, 161, 162, 164. PW1600/10 - XRA157, 159, 161, 162, 163, 164
1. Software for XRF	
2. PW1490/75 Functional differences between version 3.2 and 3.1 of X14 (RSX11-M).	Replace software
3. CRISS software for XRF11	New software

1. SOFTWARE FOR XRF

1.1. PW1490/ .. SOFTWARE PACKAGE (X14).

CPU	Monitor	Medium	Version	Release date	Update number	Firm ware (μproc) prerequisites version	Remarks
/00 P851	FRTM	Single density disc	02.0	05-10-79	–	2.0	old
			02.1	10-03-80	9430 900 85001	2.0	old
			02.2	26-09-80	9430 900 85031	2.0	old
			02.3	30-01-81	9430 900 85111	2.0	new
/40 PDP11	RT11-SJ	Single density disc	03.0	15-08-80	9430 900 85021	2.0	old
			03.1	24-02-81	9430 900 85151	2.0	new
/41 PDP11	RT11-SJ	Double density disc	03.1	24-02-81	9430 900 85131	2.0	new
/45 PDP11	RT11-SJ	RL01 firm disc	03.0	09-10-80	–	2.0	old
			03.1	24-02-81	9430 900 85171	2.0	new
/50 PDT11	RT11-SJ	Single density disc	03.0	19-08-80	9430 900 85061	2.0	old
			03.1	24-02-81	9430 900 85181	2.0	new
/74* PDP11	RSX11-M	RK05 firm disc	–	–	–		
/75 PDP11	RSX11-M	RL01 firm disc	03.1	13-02-81	–	2.0	old
			03.2	05-05-81	9430 900 85201	2.0	new
/76* PDP11	RSX11-M	RL02 firm disc	–	–	–		

* available second half of 1981

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2. FUNCTIONAL DIFFERENCES BETWEEN VERSION 3.2 AND 3.1. OF X14 (RSX11–M).

2.1. COMMAND ASP (ASSEMBLE SYSTEM PARAMETER) IS ADDED.

With the ASP command, one can change the vector-address and the external page address. The two addresses will be included in the system parameter file "SYS PAR. DAT".

2.2. CHANGING THE DL11E VECTOR- AND EXTERNAL PAGE ADDRESS.

The DL11E vector- and external page address can be changed inside the XRF software package, by proceeding as follows:

:

a. Delete any SYSPAR. DAT file present on the disc
b. Type XRF in order to initialise the XRF package
c. Answer the questions
d. Type RUN PW1400
e. After the message "*** NO SYSTEM PARAMETERS ON SY0:", type a carriage return for all questions, until the question "DL11E VECTOR ADDRESS" arises. Typing a zero now will switch the XRF-package off-line, so that the spectrometer is not connected and ANALYSIS commands can not be processed. The other program parts such as ASSEMBLY, UPDATE and HWTEST can still be used.
   Typing a carriage return for this question, and the following, will save the vector address "300 and the external page address "175610 in the system parameter file and the spectrometer will be connected to these addresses.
   Typing another address and/or external page address, will save that/these address(es) in the system parameter file, whereafter the spectrometer will be connected to these addresses.
   After that the following questions can be answered with a carriage return.

   After such a system parameter file has been saved on disc, it is possible to change features in this file by giving the ASP command. The same questions will be asked now; typing another address or zero as answer on the DL11E question(s) will not influence the current PW1400 run; these new addresses will be valid after the current PW1400 session has been terminated with the command END, and the XRF package has been restarted with the RUN PW1400 command. It is not necessary to delete the system parameter file now; this is only required the very first time that the XRF package has been started from a disc.

   E.g.:

```
*** NO SYSTEM PARAMETERS ON SY0:
TERMINAL TYPE = PR      := < input or cr, see users guide >
SYSTEM OPTIONS= 0       := < input or cr, see users guide >
CONCENTRATION AND LISTING OUTPUT DEVICES:
1 = TT    := < input or cr, see users guide >
WIDTH = 72    := < input or cr, see users guide >
2 = TT    := < input or cr, see users guide >
WIDTH = 72    := < input or cr, see users guide >

START TRANSM. CODE    =    0 := < input or cr, see users guide >
END   TRANSM. CODE    =    0 := < input or cr, see users guide >
DL(V)11–E VECTOR      =    300 := type address, zero or < cr >
DL(V)11–E ADDRESS     =    175610 := type address or < cr>

NR OF IDENT FIELDS = 1 := < input or cr, see users guide >
FIELD WIDTH 1 = 20 := < input or cr, see users guide >
TEXT1 = IDENT     := < input or cr, see users guide >
```

2.3. SEE XRA–164 FOR:

- Description of starting up the RSX11-M, and the XRF software
- Generation of the RSX11–M operation monitor.

3. CRISS SOFTWARE FOR XRF11 (X14 AND X16)

We have signed a licence agreement with Criss Software Inc., which enables us to offer the Criss fundamental parameters calculation method in our software, under the following type numbers.

3.1. PW1599/.. SOFTWARE PACKAGE (X14 AND X16)

CPU	Monitor	Medium	Version	Release date	Update number	Firm ware (μ-proc) prerequisites version	Remarks
/40 PDP11	RT11-SJ	Single density disc	–	05-05-81	–	–	New
/41 PDP11	RT11-SJ	Double density disc	–	05-05-81	–	–	New

3.2. INTRODUCTION

The Criss software is an off-line package used for the theoretical calculation of matrix effects in XRF sample analysis, using the D.E.C. PDP11 series of minicomputers (with the RT11 operating system).

NOTE: that it will never be available with the P800 series minicomputers.

The licence to use the software has to be purchased, and we have to pay a licence fee for every copy sold to an end-user. Therfore the N.V. Philips parties and the end-user must sign a "User Agreement" prior to the shipment of the package.

3.3. DESCRIPTION OF THE SOFTWARE PACKAGE

The following text describes the software, and is taken from the Criss brochure.

XRF-11 is user-oriented software for eliminating interelement absorption and fluorescence effects in XRF data.

Automatic processing can be used, as well as interactive operation, depending on the desire for analyst intervention at run time. Data and commands can be read from user files.

Accurate analysis requires very few standards. In many cases, just pure elements or oxides, or even a single type standard, produce the same accuracy as the older empirical methods, which often required a dozen or more different reference standards. XRF-11 can be used without measurements of any standards at all, once the spectrometer system is calibrated for the elements of interest. However, the greatest accuracy is obtained when one or more standards are measured to determine the instrument response levels.

Calibration curve shapes are determined automatically from calculations based on such fundamental parameters as x-ray absorption coefficients, fluorescence yields, Auger and Coster-Kronig transition probabilities, and other data provided with XRF-11 and accessed automatically as needed. The x-ray tube output spectrum, including lines and continuum, is calculated from an accurate, efficient mathematical model. XRF-11 can also treat specimens excited by isotopes or fluorescers. Matrix absorption and secondary fluorescence calculations use well-established formulas developed by Sherman, Gillam and Heal, Shiraiwa and Fujino, and others for thick, homogeneous specimens. XRF-11 uses a thin-sample correction from the work of Compton. Novel numerical techniques are used to speed the calculations and make theoretical predictions conform to whatever standards are available.

Additional features of XRF-11 include treating oxides and other compounds as the independent components of interest, fixing the amounts of fluxes, internal standards, and other known constituents, calculating an un-measured component by difference, fine-tuning and procedures to balance speed vs. accuracy, and outputting intermediate results if desired.

XRF-11 is the only laboratory software with these state-of-the-art capabilities. Until the first version of XRF-11 was announced in March, 1979, such elaborate calculations were possible only on large main-frame computers. XRF-11 was described, with test results, in a paper at the 1979 Denver X-Ray Conference (see *Advances in X-Ray Analysis*, Vol. 23, Plenum Publishing Corporation, 1980, pp. 93-97).

You will find that some analysts support this statement, but others object to it. We now know that as more standards are added to XRF11 the unknown samples calculation becomes more accurate, almost as accurate as using our theoretical alphas with the same number of standards. However; the main advantage of using the Criss package is that it gives the user the possibility to get concentrations from samples outside the normal calibration ranges, or to get concentration estimates from completely unknown samples.

We have made some Philips specific modifications to the Criss package, to facilitate automatic access to measurements data written to disc files by our standard software packages; and further modifications are in hand.

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820721 SOFTWARE SURVEY NO. 5 XRA189

PW1400/00 – PW1600/10

Subject:	Action required:
	Already issued: PW1400/00 – XRA141, 142, 150, 153, 156, 157, 161, 162, 164, 167, 169, 178, 179, 180, 181, 183.
	PW1600/10 – XRA157, 161, 163, 164, 167, 169, 171, 172. 173, 177, 180, 185.
1. Software update numbers	Note
2. PW1490/75/76 Functional differences between versions 4.1 and 4.0 of X14D (RSX11-M).	Replace software
3. PW1690/75/76 Functional differences between versions 2.0 and 1.1 of X16D (RSX11-M)	Replace software
4. Start up of the X16D and X14D software, including insertion or change of vector and page address information.	

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1. SOFTWARE UPDATE NUMBERS

The system of giving a separate update number for each new release of software has now been discontinued, and in future the order number given below will automatically be supplied as the most recent version.

PW 1490/.. Software package (X14)

CPU	Monitor	Medium	Version	Release date	Update number	Firm ware (μ-proc) prerequisites version	Remarks
/00 P851	FRTM	Single density disc	02.0	05-10-79	—	2.0	old
			02.1	10-03-80	9430 900 85001	2.0	old
			02.2	26-09-80	9430 900 85031	2.0	old
			02.3	30-01-81	9430 900 85411	2.0	new
/40 PDP11	RT11-SJ	Single density disc	03.0	15-08-80	9430 900 85021	2.0	old
			03.1	24-02-81	9430 900 85421	2.0	new
/41 PDP11	RT11-SJ	Double density disc	03.1	24-02-81	9430 900 85431	2.0	new
/45 PDP11	RT11-SJ	RL01 firm disc	03.0	09-10-80	—	2.0	old
			03.1	24-02-81	9430 900 85441	2.0	new
/50 PDT11	RT11-SJ	Single density disc	03.0	19-08-80	9430 900 85061	2.0	old
			03.1	24-02-81	9430 900 85451	2.0	new
/74 PDP11	RSX11-M	RK05 firm disc	No longer advised				
/75 PDP11	RSX11-M	RL01 firm disc	03.1	13-02-81	—	2.0	old
			04.0	15-12-81	9430 900 85471	2.0	old
			04.1	25-03-82	9430 900 85471	2.0	new
/76 PDP11	RSX11-M	RL02 firm disc	04.0	15-12-81	9430 900 85481	2.0	old
			04.1	25-03-82	9430 900 85481	2.0	new

PW 1690/.. Software package (X16)

C.P.U.	Monitor	Medium	Version	Release date	Update numbers	Firm ware (μ-proc) prerequisities version	Remarks
/00 P851	FRTM	Single density disc	02.0	23-05-80	—	2.1	old
			02.1	10-10-80	9430 900 85091	2.1	old
			02.2	15-01-81	9430 900 85121	2.1	old
			02.3	04-09-81	9430 900 85611	2.1	new
/40 PDP11	RT11-SJ	Single density disc	01.1	15-08-80	9430 900 85041	2.1	old
			01.2	24-02-81	9430 900 85621	2.1	new
/41 PDP11	RT11-SJ	Double density disc	01.2	24-02-81	9430 900 85631	2.1	new
/45 PDP11	RT11-SJ	RL01 firm disc	01.2	24-02-81	9430 900 85641	2.1.	new
/50 PDT11	RT11-SJ	Single density disc	01.1	05-08-80	9430 900 85071	2.1	old
			01.2	24-02-81	9430 900 85651	2.1	new
/75 PDP11	RSX11-M	RL01 firm disc	01.1	09-09-81	—	2.1.	old
			02.0	11-03-82	9430 900 85671	2.1	new
/76 PDP11	RSX11-M	RL02 firm disc	01.1	09-09-81	—	2.1.	old
			02.0	11-03-82	9430 900 85681	2.1	new

2. PW1490/75/76

Functional differences between version 4.1 and 4.0 of X14D (RSX-11-M)

.1 Sometimes asterisks were printed in output fields, where numbers should have been printed. The conversion of the number to the ASCII print string has been changed.

.2 The MCF command (Measure samples according to the sample Changer File, using the HERZOG automatic sample changer) could be given by the operator, while the microprocessor was still busy with a previous command, which is wrong. In this version the MCF command is forbidden, if the spectrometer is still busy.

.3 The ATI/PTI command (Assemble/Print Tray Identification), given during a measurement, could reset the current measurement. This is corrected.

.4 The copyright message is printed when starting the X14D package.

3. PW1690/75/76

Functional differences between version 2.0 and 1.1 of X16D (RSX-11-M)

.1 If the spectrometer is busy and a command is partially typed in by the operator (without giving <CR>), it will be aborted after 10-20 seconds, and the X16D package will show this with a ^U after the aborted command.

This is necessary for organisational reasons.
The same procedure is valid for commands entered after the *MAN command has been given (commands for microprocessor).

.2 Some errors have been corrected in this version:

.2.1 If the command SMX nn O. was sent to the microprocessor, it was erroneously converted to SMX nn 1.

.2.2 In the regression program if the command SRA (Start Regression Analysis) is used, and 10 alphas have been included as correcting elements, an error message ERROR 10 occured. Up to 20 alphas can be fixed in a regression analysis calculation, and up to 10 alphas can be calculated (by giving CAL EL) in an SRA routine.

.2.3 The DL11E vector - and the external page address questions have been removed from the ASP command (Assembly System Parameters). These will only be asked if the spectrometer is put on-line or off-line. The DL11E addresses will be asked the first time that the disc containing the X16D package is booted, and these will be built into a spectrometer driver, which contains certain features of the executive. This is necessary, as the driver tables are an implicit part of the executive.

Also refer to paragraph 4

4. START UP OF THE X16D AND X14D SOFTWARE, INCLUDING INSERTION OR CHANGE OF VECTOR AND PAGE ADDRESS INFORMATION.

The terminal output during the "start up" procedure of the X16D software is given below, showing input required by the operator. The procedure for the X14D software is similar.

This output is followed by the procedure required when an existing vector and page address input must be changed. In this case the sequence driver files SQDRV. TSK;1 and STB; 1 must be deleted.

```
000020 000001 000550 003774
@DL

  RSX-11M V3.2 BL26   124K   MAPPED
>RED DL:=SY:
>RED DL:=LB:
>MOU DL:RSXM26
>@DL:[1,2]STARTUP
>* Enter date and time ( dd-mmm-yy hh:mm ) [S]: 7-JUL-82 12:48
>TIM 7-JUL-82 12:48
  !
  ! ...Working...
  !
  ! ... Ignore any message FILE NOT FOUND or NO SUCH FILES ...
  !
INS -- FILE NOT FOUND
  !
  ! ... Working ...
  !
PIP    NO SUCH FILE(S)
  !
    The X16 package uses a DL11E driver called SQ:, and this driver is
  ! not yet present on the disk.
  ! It will be assembled and linked now, using the features of the
  ! executive on LB0:.
  ! After linking this driver, it must be made known to the executive
  ! by booting the system another time.
  !
  * Vector for DL11E (default=  300) [0]: 330
  * CSR    for DL11E (default=17756[0) [0]: 175630
  !
  ! ... Compiling the SQ: driver tables ...
  ! ... Compiling the SQ: driver body   ...
  ! ... Taskbuilding the SQ: driver     ...
  ! ... Unload any old SQ: driver       ...
  !
  ! *** The system will now be booted again to insert the new driver
  ! *** tables into the executive
  !
  * Ready for software booting (default=NO)? [Y/N]:Y
BOO [1,54]RSX11M

  RSX-11M V3.2 BL26   124K   MAPPED
>RED DL:=SY:
>RED DL:=LB:
>MOU DL:RSXM26
>@DL:[1,2]STARTUP
>* Enter date and time ( dd-mmm-yy hh:mm ) [S]: 7-JUL-82 12:55
>TIM 7-JUL-82 12:55
  !
  ! ...Working...
  !
  ! ... Ignore any message FILE NOT FOUND or NO SUCH FILES ...
  !
  !
  ! If the PW1690/.. executive is used and the users configuration is
  ! a PDP 11/23 with DL11J interface, only TT0: can be used as terminal;
  ! else TT0: and/or TT1: can be used as terminals.
>!
>* What is the highest terminalnumber in use (default=0) [0 0:0]: 1
  !
  ! ...Setting the terminals...
  !
  ! ...Acknowledge all terminals...
  !


  07-JUL-82 12:55          FROM TT0:       TO TT0:
  TO ENTER THE SYSTEM, TYPE HEL SYSTEM/SYSTEM


HAVE A GOOD AFTERNOON
07 JUL 82 12:55 TT0:  LOGGED OFF

@ <EOF>
```

```
>HEL SYSTEM/SYSTEM

        RSX-11M BL26   MULTI-USER SYSTEM

GOOD AFTERNOON
07-JUL-82 12:55 LOGGED ON TERMINAL TT0:

>@LOGIN.CMD
  ! ! /ID/ f1:
  ! ! this terminal a CRT? [Y/N]:N
  ! ! we X14 to initialise the X14 package
  ! TYPE X16 TO INITIALIZE THE X16 PACKAGE
  ! ! or HEL- on XRF package, type HELP
  @ EOF
  X16
  ; STARTING UP THE X16 - PACKAGE
  ;
  ; default settings are :
  ; Task on - DL0:202,54
  ; Data to - DL0:202,54
  ; Terminal T1 = TT1:
  ; Terminal T2 = TT1:
  ; Terminal T3 = TT1:
  ; Terminal RT = TT1:
  ;
  * Do you want above settings (default=NO)? [Y/N]:
  ;
  ; If any question is not clear, type HELP as answer on that question
  ; If a wrong answer has been given on a question and the <cr> has
  ; not yet been given for that answer, the answer can be erased by
  ; typing CTRL-U (control key and U key simultaneously).
  ; If a character must be erased, use the DELETE key.
  ; If the entire X16 sequence must be aborted, type control-Z as
  ; answer on a question.
  ;
  * Octal UIC-membernumber for X16-package; default=54 (nnn/HELP)?: [S]:
  !
  ! If (a) warning(s) INS -- ILLEGAL DEVICE xxn: occurs, the indicated
  ! device(s) xxn: are not included in the system configuration and
  ! must not be used in the X16D package
  !
INS -- ILLEGAL DEVICE LP0:
>
INS -- ILLEGAL DEVICE LP0:
INS -- ILLEGAL DEVICE TT2:
INS -- ILLEGAL DEVICE TT3:
;
  * Device for X16 data files; default=DL0 (ddu/HELP)? [S]: DL1
>* Is there a FILES-11 medium present in DL1: (Y/N/HELP)? [S]: Y
>* Is unit DL1: ready to be mounted;default=NO (Y/N/HELP)? [S]: Y
>* Octal UIC-membernumber to write data files to; default=54 (nnn/HELP)? [S]: 66
>!
>! Any message DIRECTORY ALREADY EXISTS can be ignored
>!
UFD -- DIRECTORY ALREADY EXISTS
UFD -- DIRECTORY ALREADY EXISTS
;
>; Terminal assignment section
;
; Standard terminal assignments are :
>; Device T1 = TT1:
;         T2 = TT1:
; ;       T3 = TT1:
;         RT = TT1:
;
  * Any changes; default=NO (Y/N/HELP)? [S]:
  ! ********************************************************
  ! ***** STARTED AT                 : 07-JUL-82  12:58:25
  ! ***** X16 TASK FILES ON           : DL0:[202,54]
  ! ***** X16 DATA FILES ON (SY0,SY1) = DL1:[202,66]
  ! ***** TERMINAL T1                : TT1:
  ! ***** TERMINAL T2                : TT1:
  ! ***** TERMINAL T3                : TT1:
  ! ***** TERMINAL RT                : TT1:
  ! ********************************************************
  ;
  ; ***** TO CHANGE FEATURES OF ABOVE LIST, TYPE: >X16
  ;
  ; ***** TO RUN THE X16    SOFTWARE PACKAGE, TYPE: >RUN FW1600
  ; ***** TO RUN THE REGRES SOFTWARE PACKAGE, TYPE: >R16
  @ <EOF>
```

```
>RUN PW1600

X16D-002.0 RSX11M

*** ERROR D4

*** NO DATABANK IN MEMORY

*** NO SYSTEM PARAMETERS ON SY0:
TERMINAL TYPE= PR    :=
SYSTEM OPTIONS=   0 :=
CONCENTRATION AND LISTING OUTPUT DEVICES :
 1 = TT    :=
WIDTH =   72 :=
 2 = TT    :=
WIDTH =   72 :=
START TRANSM.CODE=       0 :=
END   TRANSM.CODE=       0 :=
SPECTROMETER ONLINE = YES :=
NR OF IDENT FIELDS = 1 :=
FIELD WIDTH 1 = 20 :=
TEXT1 =IDENT     :=

SQ-DRIVER V2.0,VECT=     330,CSR= 175630
** RAMS TESTED

** ADDRESS F0 F1 E0 B0 D1 70 60 80 81 83 87 8B 8D 8F

** STATUS  9A D5 80 83 02 4C 4A 82 82 82 82 82 82 82

** ERROR FRAMING

** ERROR OVERRUN

** PW1600 (VS2.2)

** PROMS TESTED

** RAMS TESTED

** ADDRESS F0 F1 E0 B0 D1 70 60 80 81 83 87 8B 8D 8F

** STATUS  9A D5 80 83 02 4C 4A 82 82 82 82 82 82 82

** ERROR OVERRUN

** PW1600 (VS2.2)

** PROMS TESTED

** RAMS TESTED

** ADDRESS F0 F1 E0 B0 D1 70 60 80 81 83 87 8B 8D 8F

** STATUS  9A D5 80 83 02 4C 4A 82 82 82 82 82 82 82

* WDB PW1600

*

 HEL SYSTEM/SYSTEM

        RSX-11M BL26   MULTI-USER SYSTEM

GOOD AFTERNOON
07-JUL-82 12:49 LOGGED ON TERMINAL TT0:

 @LOGIN.CMD
>SET /FDX=TI:
>* Is this terminal a CRT? [Y/N]:N
>!Type X14 to initialise the X14 package
 !TYPE X16 TO INITIALIZE THE X16 PACKAGE
>!For HELP on XRF package, type HELP
>@ <EOF>
>UIC 1,54
>DEL SQDRV.*
DELETE FILE    DL0:[1,54]SQDRV.TSK;1              [Y/N/G/Q]? Y
DELETE FILE    DL0:[1,54]SQDRV.STB;1              [Y/N/G/Q]? Y
```

Now re-boot the system and proceed as above to input new vector and page address.

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830214 | PW1400/00 | XRA203

Action Required:

Replace firmware (microprocessor)

Already issued:

XRA141, 142, 150, 153, 157, 161, 162, 164, 167, 169, 178, 179, 180, 181, 183, 189, 196, 198, 200, 201, 202.

Product: PW1400/00 microprocessor, version 2.1.

Medium: PROM

NOTES: 1. Copies of this new release for existing customers can be ordered through:

Mr. B. Oude Lansink
S&I Logistics
Nederlandse Philips Bedrijven B.V.
Lelyweg 1
7602 EA Almelo
The Netherlands.

Ordering code: *9430 900 85401*

Price: *Free of charge (we will charge when V2.1. is shipped, and credit you when the old PROM is returned).*

Please specify on your order the customer name, and the spectrometer serial number.

2. *The new microprocessor software version has to be introduced in all equipments. Units with a serial number higher than DY1025 are delivered with the new microprocessor version 2.1.*

3. *The modified software (version 2.1.) is arranged to operate with the software programs (PW1502/00 or PW1502/40) which are necessary when a Philips or a Herzog sample changer is installed with the PW1400.*

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GENERAL DESCRIPTION OF THE MODIFICATIONS

1. **The software version number typed during the switch-on (or reset) of the software is "VS2.1".**

2. **Possible deadlock situation if a slash and c.r. is typed during the evacuation of a sample in the airlock.**

If a command is typed that results in the loading of a sample (e.g. SLP, SMP. SMX), and vacuum is then selected after the cap has gone down, and before the plunger goes down, there is a time (typically 3 ... 25,5 sec.) where the "airlock" is evacuated.
If, during that time a slash (plus c.r.) is typed to abort the requested action, a deadlock situation occurs where neither the cap or the plunger can be moved.
This situation cannot be cleared, by the software, and even by a "reset" (the red button).
The only way to remove the deadlock was to switch off/on the mains power (then the error was automatically removed).
Another way was to use a special sequence of "TST"-commands.

The software is now changed so that the abort action which is given by a slash and c.r. is delayed until the complete cap/evacuation/plunger cycle (for loading or unloading) is completed.
The slash and c.r. can still be typed at any time as required.

3. **Possible deadlock situation with a P-800 series Philips minicomputer connected to the PW1400**

If the transmission of information from the PW1400 microprocessor to the minicomputer goes too fast for the mini, the handshake lines can be used by the mini to suspend the transmission from the micro. This works quite well in the DEC PDP-11.
The interface-card in the Philips minicomputer however does not work too well in the full duplex mode, it can only switch the handshake lines when it is in the transmit-mode.
To give the mini the time to switch from the receive mode to the transmit mode, and not losing characters, there is a delay of 100 milliseconds after each line of output from the PW1400, during which time the mini can carry out the action.
An output line is defined as a string of characters ending with a carriage return, so after each carriage return there should be a delay.

This delay was not implemented in an "empty line" (l.f. c.r. only) which is transmitted before (!) "C=" and error-messages.
This resulted in the possibility that with long messages, and mostly when a (slow) printing device was used as the operators terminal for the mini, there could occur a deadlock situation.
If the mini is switched from receive to transmit just after the carriage return before the C=, the "C=" characters sent by the PW1400 were missed, and the PW1400 carries on waiting for the characters.

In the new micro-software this delay is now given after **each** carriage return is transmitted.

4. **Error in scan length on the recorder paper**

If during a continuous scan a diagram is written by the recorder, the length of this scan, measured in time, is about 0,2 seconds too long.
With the maximum recorder speed of 8 cm/minute this is about 0,3 mm of chart length. Additionally this error is cumulative, so that after a few scans the recording is visibly too long.

In the new software this 0,2 second error is removed.

5. **"** ERROR BATTERY, PARAMETERBANK CLEARED", without battery error**

Sometimes, when the power of the PW1400 is switched off, the power-down reset for the microprocessor does not work properly. This can result in erroneous information in the RAM.

In many cases most of the CPU time is spent on testing status words in the RAM (e.g., in C= mode and during measurement).
If a faulty power-down occurs, this reading of specific RAM addresses can affect the writing (!!!) to (other) addresses. In most cases this is only in the "scratch" area, but sometimes real information is destroyed.
When the PW1400 is powered up again there is a test of the validity of (some) RAM addresses, and if these are changed the software assumes this is due to an improper battery, clears the RAM and generates the error-message: "** ERROR BATTERY, PARAMETERBANK CLEARED".

In the new software the two most executed "wait-loops" (C = / measurement) are not executed continuously, but the processor is put in a "HALT", from which it is wakened by each interrupt. This happens after at least each 100 milliseconds, and with each keyboard input.

If the power is switched off when the processor is in a "HALT" situation there is no erroneous writing to the RAM. The error rate is improved by 100 ... 1000, and is not detectable any more.

6. **USART restartable without hardware reset**

When the microprocessor starts (at address 0000 H) one of the first actions is to program the USART's (serial I/O chips) for baud rate, parity, etc.
In the method selected this programming must be preceeded by a hardware reset, as is done with "power off/on", or the "reset-button".
If the software was (re) started by means of a "TST E 0000" command; or a "jump 0000" in a test program, this hardware reset was not present and the programming of the chips went wrong and there was no communication with the operators terminal any more.

In the new software version another method is chosen to progam the USART's, and the hardware reset is not required any more.

7. **"Test bus" test command ends with all output lines low instead of high**

If a HERZOG sample changer/loader is to be connected to the PW1400, there is a test possibility to check the "PHILIPS" part of the installation.
The delivered short-circuit plug can be used to connect all the output lines from the sample changer interface card in the PW1400 to all the input lines (can be done on the sample changer connection plug).
With the command "TST B C080 C080 FF" the micro-processor now automatically tests the interface card and the cabling.
However, after the test all output-lines are "high", and if without switching the PW1400 off, the HERZOG sample changer is connected, all functions of the changer are activated at the same time. This was not an acceptable situation.
By using the test command "TST W C080 00" this situation could be corrected.

In the new software the test is changed in such a way that after the test all output lines are "low".

8. **Switching from a 72-position sample changer to a 6/12 position loader could result in a deadlock situation**

In the rare situations were a PW1500/15, /16 (72 position) is replaced by a PW1500/05, /06 (loader) there could be a deadlock situation where the software waits for the depression of a microswitch which is not present in the loader.

The test command "TST W 40D5 00" could solve this problem.

In the new software this problem is solved in the "start-up" procedure, so that it is automatically done at power on (or "reset")'

9. **Ratemeter selection after power on**

If the PW1400 starts up, the ratemeter (RMS) was not selected by the software, nor by the hardware, and thus was random. This could also result in an erroneous display of the ratemeter setting.

The software is modified now so that the RMS after power up will be the same setting as it was when the power was switched off.

Only for the first time, and after an "** ERROR BATTERY", the selection will be "manual" (not user selectable !).

10. **Improvement of the KVM - instruction**

Generator "MANUAL" can be selected by the operator of the PW1400 if a zero is typed for one, or both of the two arguments in the "KVM kV, mA" - instruction (e.g., "KVM 30,0" or "KVM 0,0").
If a valid kV value was typed and the mA value was not typed (e.g. "KVM 30"), then the microprocessor assumes mA=0, thus resulting in the selection "MANUAL". This should be avoided if the generator is already set at a high kV and/or high mA value.

The KVM instruction is now changed so that an error-message is generated ("** INVALID ARGUMENT"), and the previous kV, mA setting is not changed.

11. **Removal of "dead-code"**

There existed a small part of a so-called "dead-code" i.e. a code that is not used any more, but is still present in the memory. (This had no external effects).
This is now removed.

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830501 PW1400/00 Spectrometer with HP85A Software Package XRA 209

Already issued: XRA 141, 142, 150, 153, 157, 162, 167, 169, 178, 179, 180, 181, 183, 189, 196, 198, 201, 203, 206.

Subject	*Action required*
Software package for a HP85A Calculator connected to a PW1400/00	– 1 Ordering information and functional differences. – 2 Add Description, Installation, and User instructions to the PW1400 Service Manual.

1 ORDERING INFORMATION

The updated software package (version 2.0) can be ordered from:
Mr. B. Oude Iansink
S&I Logistics
Philips Export B.V.
Lelyweg 1
7602 EA Almelo
The Netherlands
Ordering code: 9430 900 85301

Functional differences between version 2.0 and 1.0

Type of change	Module	Description
1 M	ST	Change version number from 1.0 to 2.0, and change of output format.
2 S	AN	Store PW1400 Parameter Bank on the HP85A tape cartridge (DPB command).
3 S	AN	Load PW1400 Parameter Bank from the HP85A tape cartridge (RPB command).
4 E	AN	System blocked because of Format error in the Recalibration Routine. Line 3090: OFF ERROR @ RETURN
5 M	AN	Monitor Update: results presentation
6 E	AN	Monitor Update: % difference calculation. Line 2670: (1 - C(3,E) /R(1,E)) *100 becomes (R(1,E) /C(3,E) -1) *100

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7 S	AS	Copy existing DP-list to any tape cartridge. Line 245: ON KEY # 3 , "DPcopy" GOTO 385 Line 385: F1=1 @ GOTO 210
8 M	AN	Read from tape rearranged. Lines 660 through to 690
9 M	AN	Line 835: FO=O @ GOTO 220 ! Return to manual operation. Line 840 through to 1010 rearranged, using line 835
10 E	AS	Damaged DP - list after using soft key "Index" with DP - list present.
11 M		File names throughout package are changed as follows: – File "8514AS" becomes "1400AS" – File "8514AN" becomes "1400AN"
12 M		Add subroutine CLEAR SOFT KEYS and remove any OFF KEY statements.
13 M	AS	Option selection in subroutine "DISP/EDIT DP HEADER" is reorganised.
14 M	AS	Review of spectral sets is reorganised.

Type of change.
(M=Modification, S=Specification, E=Error).
Module which was changed.
(ST=Autostart, AS=Assembly, AN=Analysis)

2 PW1400 SERVICE MANUAL ADDITIONS

Add the following sections to the PW1400 Service Manual, pages 4 - 152 / 153:

Description, Calculator HP85A

The software package runs on a HP85A personal computer which is connected to a Philips PW1400/00 X-Ray spectrometer. The software will communicate with the spectrometer microprocessor and convert X-Ray intensities into concentrations, using the following capabilities:

- up to 4 samples can be analysed in one run
- intensity data can be input from the PW1400, or from the keyboard
- raw data from up to 20 measurement sets can be accepted for processing
- data can be corrected for spectral interference
- calculation of internal and/or external ratio intensities is possible
- concentrations for up to 15 elements can be calculated
- inter-element correction to any or all of these 15 elements can be applied, using the concentration data from the first 10 elements.
- channel names are replaced by full names.
- print-out order is independent of the measurement sequence.
- optional calculation options include:
  - replace negative C's by zero
  - calculate the sum of the elements
  - normalise to 100%
- update of external monitor values.
- update of calibration constants.

Information to convert raw data into concentrations is assembled in Data Processing (DP) lists. Up to 30 of these lists can be stored on the HP 85A tape cartridge. A survey of the existing DP lists, or the contents of a selected list, can be printed.

The calculations which are available in the software package are as follows:

1. Kilo-counts per second
2. Background subtraction – a measured background intensity is removed from a peak countrate
3. Line overlap correction – the interfering intensity of an overlapping spectral line is removed
4. Internal ratio calculation – the net element intensity is divided by the net intensity of an internal standard line
5. External ratio calculation – the net element intensity can be divided by the stored element intensity of a reference sample line
6. Concentrations calculation – the net kcps or ratios are converted into elemental concentrations, using the formulae $C_1 = D + E \cdot R\ (1 + \Sigma\ a \cdot C)$, also $C_2 \ldots\ldots C_n$ These equations are solved by an iterative process.

A recalibration file can be stored to hold the concentration data from samples to be used in a recalibration procedure. A simple procedure is used to update the D and E instrumental values which have been stored for use in the concentration calculations. If monitor samples are used, and the values are stored for ratio calculation, a simple procedure is used to measure the monitor and update the stored intensity values.

The HP85A must be equipped with:

– ROM drawer	00085 - 15003	
– I/O ROM	82936A	
– 16 kB memory module	82903A	
– Serial Interface	82939A	(standard version)

An additional one to one RS232C cable (PW1340/00) can be added between the PW1400/00 and the HP85A interface if more length is required.

Installation

Set the jumpers and switches on the serial I/O interface number 1, refer to PW1400 service Manual page 4 - 107 and figure 1, as follows:

Action	Description
J1 - close	Connection between protective ground (101) and signal ground (102)
J2 - close J3 - open J4 - close J5 - open	Polarity of WR and RD (DBIN) signals: Active high
J6 - open J7 - open J8 - close	Pcb address, I/O Interface No1, / 9xxx
J9 - open	Connection between INTR6 and INTR7
J10 - close	Connection between protective ground (101) and logic 0V
S1 - 1 = 1 S1 - 2 = 0 S2 - 1 = 0 S2 - 2 = 1	4800 Baud
S3 - 1 = V S3 - 2 = V S4 - 1 = x S4 - 2 = x S5 - 1 = V S5 - 2 = V S6 - 1 = x S6 - 2 = x	V24 (RS232 C) mode
S7 - 1 = 1	Echo character
S7 - 2 = 0	No parity
S8 - 1 = x	Parity
S8 - 2 = 1	8 bits per character
S9 -1 = V S9 -2 = V S10 = V S11 = V	V24 (RS232 C) mode

NOTE: x = immaterial (don't care)

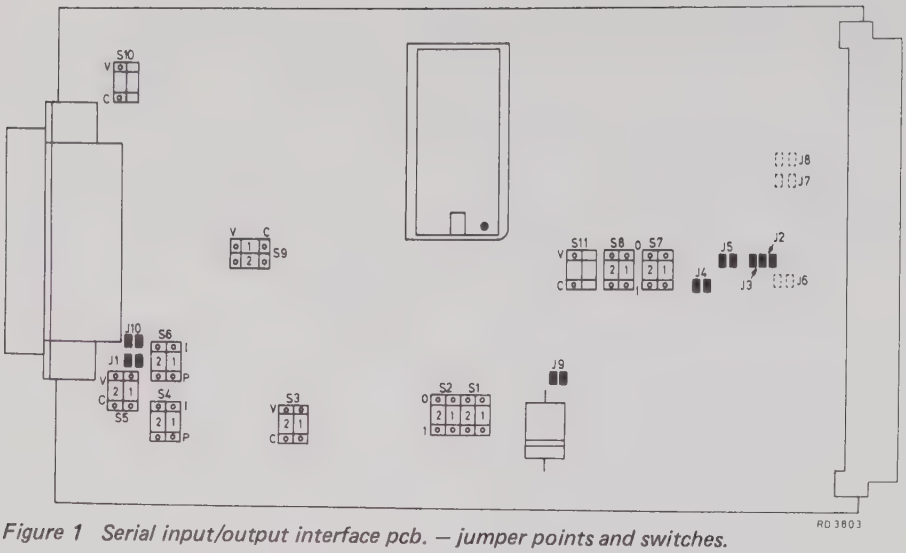

Figure 1 Serial input/output interface pcb. — jumper points and switches.

When the system is started, and the ANALYSIS module (1400 AN) is loaded — see the "User instructions" in this XRA, the HP82939A Interface hardware settings are overridden by the software, as follows:

Software input	**Action taken**
I 9 = 10	Set interface select code to 1 1 1
CONTROL I 9, 3; 13	Set baud rate to 4800, to 1 1 0 1
CONTROL I 9, 4; 7	Set character word length to 8 (1 1), stop bits to 2 (1), and no parity (0).

It is assumed that the HP interface settings are those set by HP before leaving the factory, that is:

S1 - 1 = 0	Ignore autohandshake
S1 - 2 = 1	Select code bits = 10
S1 - 3 = 1	" " "
S1 - 4 = 1	" " "
S2 - 1 = 0	No parity transmit
S2 - 2 = 0	Select add parity
S2 - 3 = 1	Enable parity
S2 - 4 = 0	1 stop bit
S2 - 5 = 1	Character word length = 7
S2 - 6 = 0	" " "
S2 - 7 = 0	Baud rate = 300
S2 - 8 = 1	" "
S2 - 9 = 1	" "
S2 - 10 = 0	" "

If it is required to check the HP interface switch settings it may be necessary to disassamble the interface housing, see figure 2. The position of the switches is shown in figure 3, which also shows the slide and rocker switches which can be fitted. Alternatively, the position of the switches can be determined by reading the status shown in table 3.1 of the HP82939A Interface Manual — which also includes a functional test description. If a different baudrate is selected the software statements should be altered or removed, and the settings should be entered in the interface hardware of the PW1400 Serial Interface. The analysis module software referring to the interface settings is shown below. The connection can be tested using soft key "X - ray", whereafter the "C=" should appear on the HP85A CRT, and then all PW1400/00 microprocessor commands can be used. If "C=" does not appear, or an error message is printed, give a HP85A reset and try again.

CAUTION: **if you change any of the factory settings, make sure that you change the proper switch segments. Do not disturb the settings of adjoining switches. Use a pencil point or similar object for changing switch settings.**

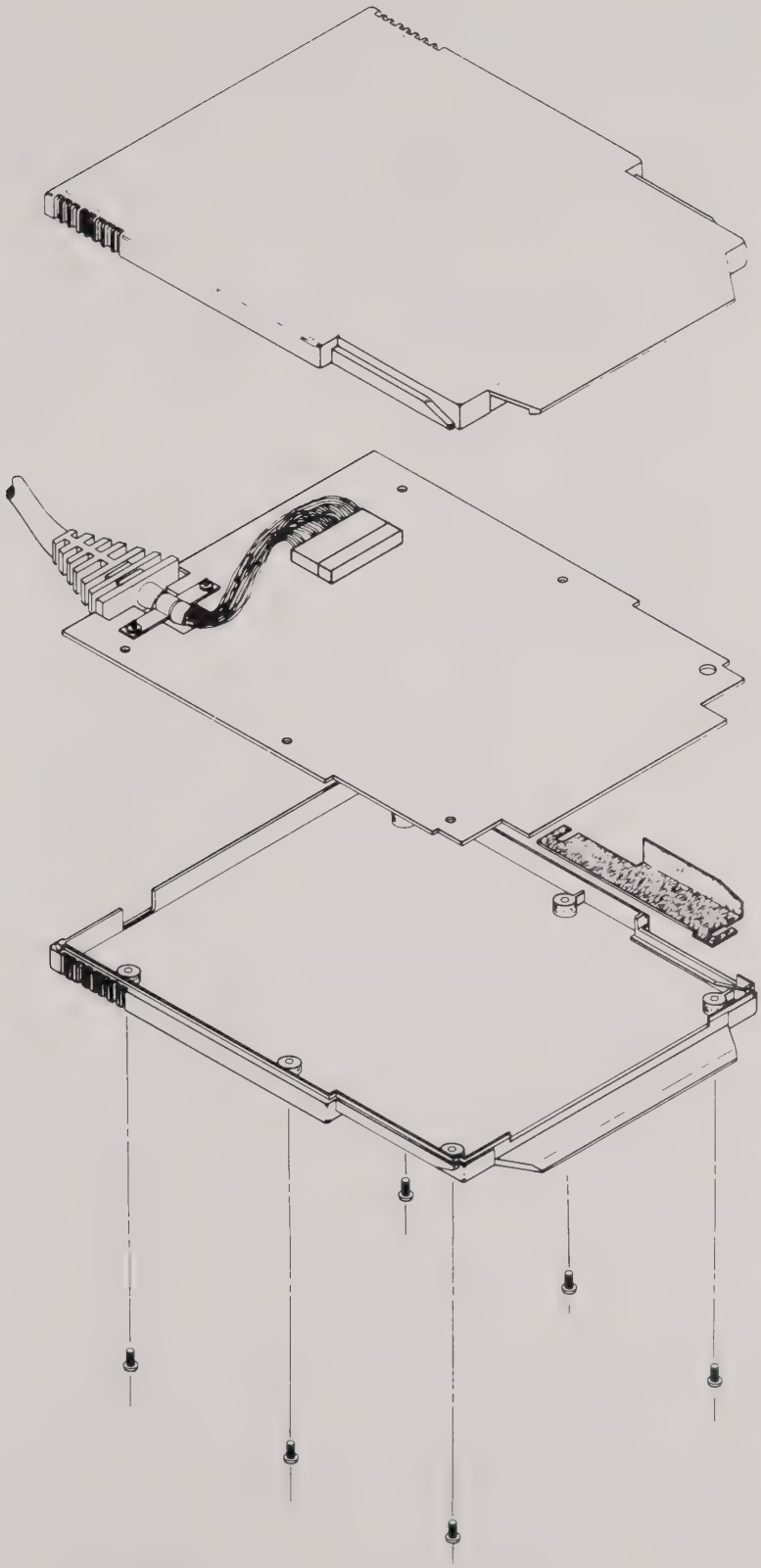

Figure 2. Disassembly of the HP Interface

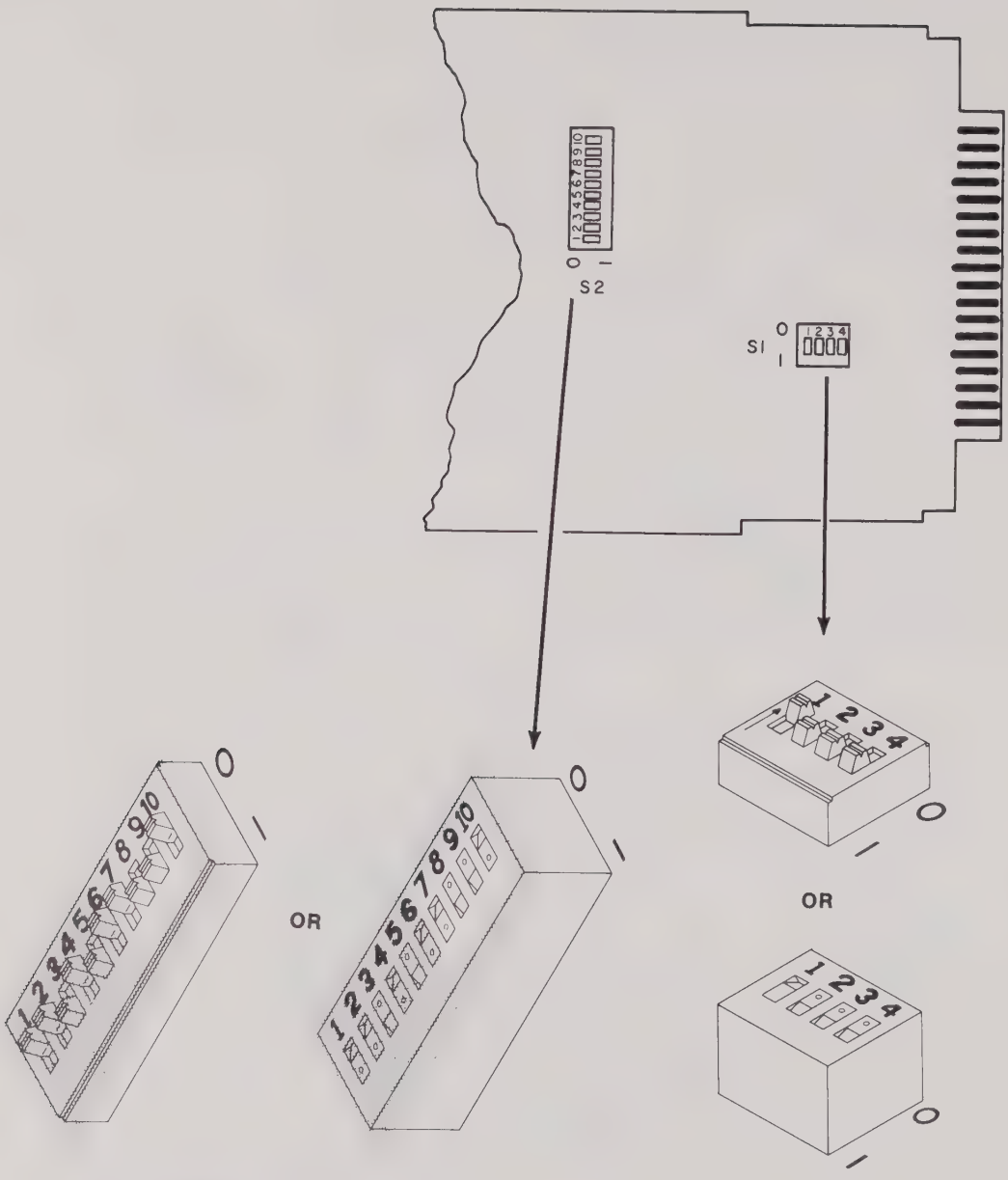

Figure 3 HP82939A Interface switch settings.

```
790 F0=1 ! Spectrometer Driver
800 I9=10 ! I/F Select Code
810 CLEAR @ STATUS I9,0 ; S@ STA
    TUS I9,3 ; S3
820 IF S#2 OR NOT BIT(S3,2) THEN
     PRINT "Use Standard Serial
    Interface!" @ GOTO 780
830 IF NOT BIT(S3,0) THEN PRINT
    "Spectrometer Off!" @ GOTO 7
    80
840 IOBUFFER Y$ @ RESET I9
850 CONTROL I9,3 ; 13 ! 4800 Bd
860 CONTROL I9,4 ; 7 ! 8b/c,2s,n
    o par
870 CONTROL I9,11 ; 6 ! Interr
880 CONTROL I9,12 ; 13 ! cr
890 CONTROL I9,13 ; 61 ! =
900 ON EOT I9 GOSUB 1020
```

Portion of the HP85A Software, referring to the HP Interface control settings.

Connect the HP85 Calculator (via its interface) to the PW1400 Serial interface connection (number 1), as shown in figure 4.

DO NOT SWITCH THE HP85A ON BEFORE THE PW1400 IS SWITCHED ON — see the user instuctions. The interfaces must be fitted before the HP85A is switched on.

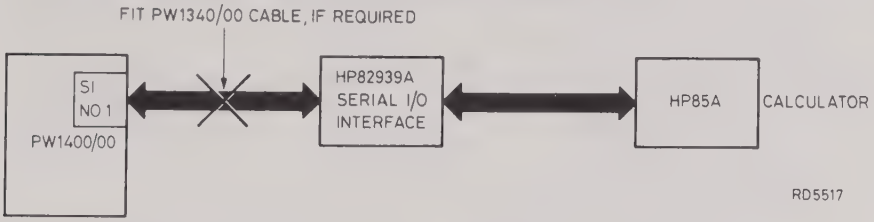

Figure 4. Connection to calculator.

Disassembly of the HP Interface housing - see figure 2

Place the interface on a flat surface with the side having the six screws facing upward and the cable coming out to the left. Then use the following steps to disassemble the interface.

1. Using a Pozidrive screwgriver, remove the six screws and set them aside.
2. Hold the interface parts together and turn it over so that the six screw holes are facing downward and the cable is still coming out to the left.
3. Hold the cable strain relief in place and remove the top half of the interface housing.

If you have followed the above steps, switch S1 should be oriented as shown in the following figure 3. If it isn't orient it as illustrated before identifying the switch segments.

When you re-assemble the interface, reverse the above procedure, making sure the ground clip is in place. The ground clip should be under the circuit board when the component side is up.

USER INSTRUCTIONS

Before using the HP85A check that the jumpers and switches of the PW1400 Serial interface board are correctly set, that the switches in the HP85A Interface are correctly set, and that the cable connections between the two units are correct.

- Switch on the PW1400
- Insert the tape cartridge system cassette in the HP85A
- Switch on the HP85A (rear panel ON/OFF switch). File "Autost" will be automatically loaded to the HP85A, and the software identification and version number will be displayed.
- The software will ask for the date, therefore type the month, day, and year. Always terminate any input with the "END LINE" key.
- The analysis module is then automatically loaded, and a "wait" instruction is output — see below.

```
Software Package

HP85A-PW1400/00

version: 2.0
   date: July 1982

Enter Date (mm.ddyyyy):=?
04.141983
Enter time (hh.mm)=?
08.56

Exit Autostart
Enter Analysis.....wait!!
```

- Input the Interface control conditions — if required.

Type I 9 = 10	Set interface select code
Type CONTROL I 9, 3; 13	Set baudrate to 4800
Type CONTROL I 9, 4; 7	Set character length to 8 characters, 2 stop bits, and no parity.

– The analysis module is checked by the HP85A BASIC Interpreter, and a menu is shown on the HP85A screen. If a DP list has not been assembled previously the redant will be as shown below:

```
= Analysis Module  PW1400/00
--------------------------------
-

# No DP-list!

##  Select Soft-Key !!



-------------------------------
SysPar
X-Ray            →DP→     DPedit
```

The assembly of a DP list and/or further action is described in the operation description of the X- ray Spectrometry Software Package, also refer to the Soft – Key Survey.

Copying a cassette

It is recommended that the system cassette, and any other original cassettes, delivered with the software package should be copied, and then kept in safe place for use as a master tape. The copied cassettes can then be used for routine operation of the HP85A/PW1400 system: Refer to figures 6 and 7.

To copy a cassette proceed as follows:

1 – Switch off the HP85A (rear ON/OFF switch)
2 – Take an empty cassette (data cartridge), check that the RECORD slide tab is in the right - most position, and insert the cassette into the HP85A.
3 – Switch on, and reset the HP85A by pressing RESET and SHIFT simultaneously.
4 – Condition the tape by typing CTAPE, < and press END LINE >. The tape runs to the end, reverses, and runs back to the start.
5 – Type the command ERASETAPE < plus END LINE >, and the tape is initialized.
6 – Catalog the tape by typing CAT < END LINE > – the tape must be empty.
7 – Remove the cassette, and the insert the system cassette.
8 – Load the "Autost" program by typing LOAD "Autost" < END LINE > . Note that lower case (small) letters are typed by holding the SHIFT key down – the opposite action to a normal typewriter.
9 – Replace the system cassette by the new (empty) cassette.
10 – Load the Autost file by typing STORE "Autost" < END LINE >.
11 – Secure/protect this file by giving the security code PH, and secure type 2; type SECURE "Autost", "PH", 2 < END LINE >.
12 – Replace the cassette in the HP85A by the system cassette again, and repeat the operations 8 to 11 above for the 1400AS program,i.e. type "1400AS" instead of "Autost". Repeat the operation for the 1400AN Program. The new cassette should now have the Autost, 1400AS (assembly) and 1400AN (analysis) programs loaded.
13 – Catalog the tape by typing CAT < END LINE >, see figure 6.
14 – The new cassette can be checked for use by:
  – Switch off the HP85A
  – Insert the new cassette
  – Switch on the HP85A - the Autost program is automatically loaded.
  – Input the date and time - the analysis program 1400AN is automatically loaded.
  – Press Soft key K4 (Special Function Key), which is DPedit in the Analysis module, and the assembly program (1400AS) is loaded.
  – Rewind the tape by pressing SHIFT and REW simultaneously.
  – The tape cassette should be removed when winding is complete, and the RECORD slide tab set to the left- hand position to protect the program data from write operations.
  – Stick a label on the cassette (similar to figure 5 - the system cassette label), and return the cassette to the protective plastic box.

SOFT KEY SURVEY

ANALYSIS module

Key #1 : X-ray	X - ray Spectrometer on - line
. key #1: /	Return to C= communication
Key #2 : Manual	Keyboard input of intensities
Key #3 : - DP -	Change DP - list
Key #4 : DPedit	Load the ASSEMBLY module
Key #5 : SysPar	Select the results output station
Key #8 : Recal	Activate recalibration routines
. Key #1 : ext.M	External monitor update
. key #2 : D, E	D and E factor update
. key #4 : ready	Return to previous soft key level

ASSEMBLY module

Key #1 : show	Show contents of DP - list
. key #1 : Elem - S	Show element set
. . key #1 : next	Show next element set
. . key #2 : back	Show previous element set
. . key #4 : ready	Return to previous soft key level
. . key #8 : edit	Edit this element set
. . . key #1 : next	Move to next component of spectral set
. . . key #2 : edit	Edit this component
. . . key #6 : delete	Delete this component from set
. key #2 : Rcal - S	Show recalibration samples
. . key #1 : next	Show next recalibration sample
. . key #2 : back	Show previous recalibration sample
. . key #4 : ready	Return to previous soft key level
. . key #8 : edit	Edit this recalibration sample
. key #4 ready	Return to previous soft key level
. key #8 : edit	Edit general header information
Key #2 : - DP -	Change DP - list
Key #3 : DPcopy	Copy DP-list to cartridge
Key #4 : Analyse	Load the ANALYSIS module
Key #5 : list	Print DP-list on HP85A printer
Key #6 : index	Print index of all DP-lists
Key #8 : DPnew	Create a new DP-list

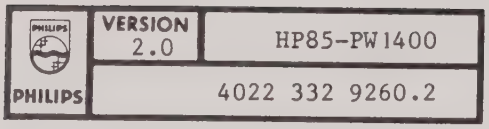

Figure 5. System cassette label

```
CTAPE
ERASETAPE
CAT
NAME     TYPE  BYTES   RECS FILE
LOAD"Autost"
STORE"Autost"
SECURE"Autost","PH",2
STORE"Autost"
SECURE"Autost","PH",2
LOAD"1400AS"
STORE"1400AS"
SECURE"1400AS","PH",2
STORE"1400AS"
SECURE"1400AS","PH",2
LOAD"1400AN"
STORE"1400AN"
SECURE"1400AN","PH",2
CAT
NAME     TYPE  BYTES   RECS FILE
Autost   PROG    256      4   1
1400AS   PROG    256     62   2
1400AN   PROG    256     94   3
```

Figure 6. Output from the copy procedure

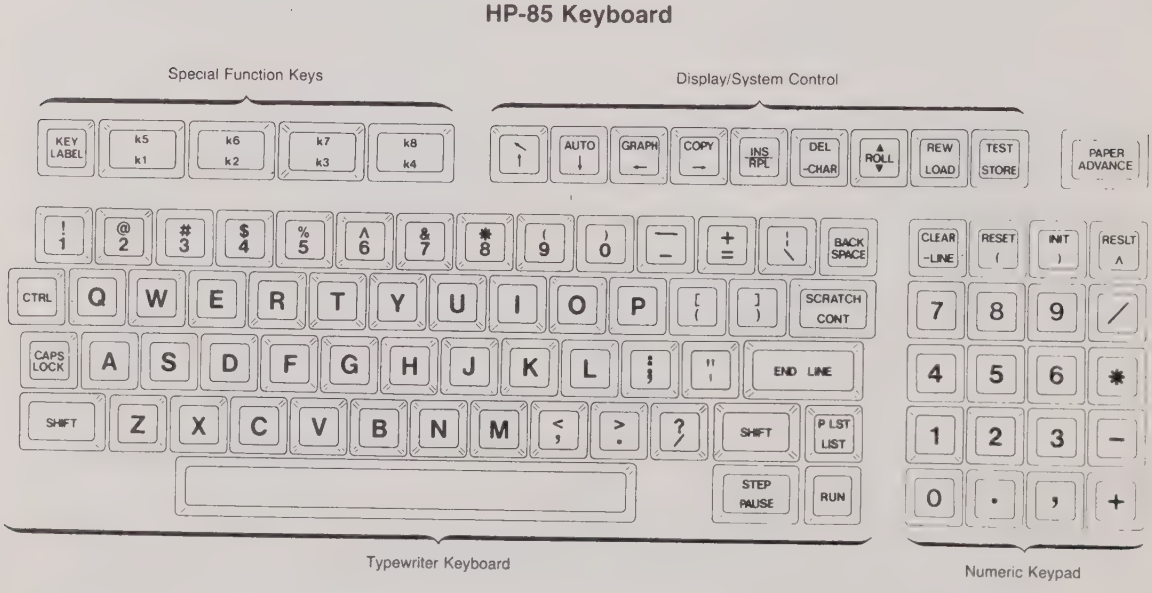

Figure 7. HP85 Keyboard

X-ray Spectrometer system
PW1400

Operation Manual

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800201

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INTRODUCTION

The PW1400 Spectrometry system is modular in design, and the basic version will measure samples according to one of the many programs which can be stored. Fully automatic analysis, with concentration calculation, is possible when a computer is added to the basic unit, and increased automation is possible with optional sample changers. Various peripheral devices can be connected for data input and output.

An H.T. generator is provided, to supply the H.T. for the X-ray tube. The range of optional accesories includes a helium flushing system.

This manual describes the operation and programming of the basic PW1400 unit, the operation and software when a data processing computer is connected, and the operation of the associated equipment and optional accessories.

Warning: X-RAYS ARE HARMFUL

The spectrometry systems produces X-rays which can be dangerous to health if the proper precautions are not taken. It is important for the health and safety of the operator that the recommendations given in the manuals be carefully observed. There must be strict compliance with local safety regulations.

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